Streamlining Life Cycle Assessment to support Ecodesign through multi-criteria materials selection

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ABSTRACT

The evaluation of the potential impact that an innovative material or technology could have on the environment, ahead of its adoption, is of fundamental importance during the design phase of a product. Life Cycle Assessment (LCA), a powerful environmental management technique, has been widely used since the mid-1980s, but two remaining problems with the methodology are its inability to allow a designer (or practitioner) to use LCA during the early design phase and the existence of uncertainties and variations in the data used in assessment.

This thesis aims to demonstrate how these issues can be solved using specific case studies as examples. The scientific content, the methodologies, and the obtained results reported here are the outcomes of projects conducted with the collaboration of two universities: Institut National des Sciences Appliquées de Lyon and Massachusetts Institute of Technology.

This thesis is divided into six main chapters:

The first chapter is dedicated to an introduction to the LCA methodology, in which it is also possible to find a literature review focused on the strengths and weaknesses that may characterize LCA. The second part of the chapter details the methods utilized to analyze uncertainty in LCA results, the state of the art for streamlined and predictive approaches and, finally, an overview of a multi-criteria analysis method useful for materials selection. In particular, the uncertainty analysis associated with LCA results may represent the starting point for the development of streamlined LCA approaches and possible methods of forecasting the environmental results of novel technologies. On the other hand, the multi-criteria analysis grounded in the uncertainty analysis presents a robust method of materials selection in support of Ecodesign.

In the second chapter, the uncertainty analysis is used to develop a streamlined LCA method founded on the *probabilistic underspecification* approach, proposed to support the building design process. The case studies analyzed in this section represent a series of residential building assemblies (exterior walls, interior walls, foundations, roofs, floors, windows, doors, exterior finishes) that were used to test the streamlined method and obtain distributions of results using a *cradle-to-gate* approach along five phases of the building design process. The bill of materials (BOM) of a building assembly can be specified using different levels of information, which can be really generic during the concept design and fully detailed during the executive project. The low-fidelity characterization of a BOM and the uncertainty associated with these low levels of fidelity are systematically quantified through probabilistic underspecification using a hierarchical classification of materials. Quantitative environmental results, processed with uncertainty analysis, were obtained using low-fidelity categories for materials and building assemblies, demonstrating that LCA can be applied not only when a complete and detailed BOM is available but also when fewer details are known.

Finally, decision-making at different stages of the design process is sustained by this approach and is based on the use of a comparison indicator.

The third chapter advances the research aimed at streamlining the LCA of buildings with probabilistic underspecification and uncertainty analysis. In particular, it investigates whether LCA can be robustly streamlined through an effective and efficient triage of data collection and the consequent selected use of specific and resource-intensive information. In this context, tests were conducted with a series of building typologies (single-family detached houses and multi-family residential buildings), again analyzed with a cradle-to-gate approach. The *probabilistic triage* approach was tested to clarify how to use probabilistic underspecification and reduce the effort involved in specification by identifying the activities that require careful characterization. With this approach, by specifying only one part of the bill of materials to the highest level of specificity, the results proved to be both reasonably accurate and obtainable with less effort. Impacts such as global warming, acidification, eutrophication, and smog creation were assessed, and the results indicated that just 40-46% of the BOM components represent 75% of the total impacts of both single-family houses and multi-family buildings.

Where the second and third chapters were devoted to the streamlined analysis of conventional products, the fourth chapter addresses the use of uncertainty analysis to forecast the environmental burden of an innovative material. Here, a scale-up protocol for an environmental impact assessment is proposed as a means to develop a streamlined *ex-ante* LCA approach. The novel element of this chapter consists of the adopted scale-up protocol. It does not rely on primary data collected by monitoring real industrial systems, as these data do not yet exist for the product of interest; instead, data measured in a plant at the pilot scale are used alongside data simulated from thermo-chemical considerations based on the stoichiometry of the considered reaction. The scale-up protocol is described and then applied to the case of polybutylene succinate (PBS), a biopolymer that is gaining attention (particularly as a replacement for polyolefins) and is obtained from bio-based succinic acid. Monte Carlo simulation was used to process the uncertainty data for all of the assessments, and a sensitivity analysis was performed to evaluate and compare the different renewable sources and chemical routes available for the production of bio-based succinic acid. The case study of PBS highlights how innovative products can be analyzed without the use of primary data, providing a way to forecast environmental impacts for novel technologies. The advantages of the adopted scale-up methodology consist of the ease of implementation and the possibility of strengthening the Ecodesign approach.

In the fifth chapter, a multi-criteria analysis was used to complete the ex-ante LCA results for PBS. The purpose of this analysis was to compare PBS to alternative materials on the basis of more than one property and for use in a specific function. This approach led to the definition of a new concept of the system boundary of the assessment: from cradle to function. The motivation for this alternative strategy stems from the application of the LCA framework to a material to obtain an *ecoprofile*: the scope of the analysis is generally from cradle to the factory gate, while the unit of mass (or volume) of the material is usually taken as the functional unit for the analysis. However, these methodological choices place relevant limitations on the effectiveness of the assessment. In this chapter, a multi-criteria materials approach was tested using the PBS results to verify and validate the environmental viability of this material's usage in packaging films. The most novel element of this research is the use of the customized *ex-ante* LCA and the uncertainty analysis, the latter of which is used to determine the uncertainty in material indices. The results were graphically represented with Ashby plots. When elongation at break and environmental performance were considered, PBS displayed a performance that was better than other traditional polyesters and comparable to the polyolefins considered; performance in terms of this set of properties is particularly beneficial in the case of secondary packaging. In the case of primary packaging, barrier properties acquire major relevance; in this regard, PBS presented among the best trade-offs for the simultaneous optimization of oxygen permeability, elongation at break and environmental impact.

Finally, the sixth chapter is devoted to the review of the approaches that were implemented and tested to streamline LCA, highlighting the strengths and weaknesses for each analyzed system and discussing future methodological developments. In particular, the uncertainty analysis based on the Monte Carlo method was used not just to characterize the quality of results but also to develop and implement streamlined approaches. Moreover, the uncertainty analysis proved to be useful for forecasting environmental results for early-stage systems and innovative materials.

In this thesis, the uncertainty analysis represents one of the most innovative and relevant points of strength from the methodological point of view. Furthermore, the use of uncertainty in environmental results allowed the characterization of an innovative material, making possible its use for multi-criteria materials selection and Ecodesign considerations.

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In memory of Prof. De Benedetti

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PREFACE AND MOTIVATION

LCA is a well-known methodology used to evaluate the environmental performance of systems, processes, and materials by assessing the environmental impacts associated with all stages of a system's life (the so-called *cradle-to-grave* approach). Once obtained, LCA results can be easily used for a range of purposes including business strategy, research and development, process design, education, policy development, product declaration and marketing (Cooper and Fava 2006). Of course, Life Cycle Assessment is characterized by a series of "unresolved problems," above all the fact that although LCA can be used as a powerful decision-making tool to explore and innovate at the R&D stage, it is generally applied by practitioners and designers at the end of the design process because of the complexity in data collection and scope definition (Reap et al. 2008; Finnveden et al. 2009). This excludes *de facto* the possibility of obtaining environmental results that can be used to drive decision making during the early concept or schematic design phase.

A streamlined approach able to facilitate the use of LCA at the early stage is crucial for the development of life cycle thinking in the design process.

Therefore, the motivation for this research is driven by the following key points:

- The need to streamline LCA to enable the use of LCA results during the different phases of the design process (for example, the design process of an innovative technology);
- The need to develop ex-ante LCA to make it possible to estimate LCA results for innovative systems (for example, an innovative material) with a certain level of confidence; and
- The need to include an uncertainty analysis in the results to lend robustness to the overall study and reliability to the hypotheses made during the LCA modeling phase.

The third key point is probably the most important element of this research, as LCA results rely on the robustness of the mathematical model. In general, the use of the Life Cycle Thinking (LCT) approach is particularly helpful for understanding the several issues that occur when a new material or technology is under development. However, the inclusion of environmental performance as an additional metric of evaluation, when one design has to be chosen from several, may be really complex.

The first project, in which LCA was used to forecast the environmental burden of an innovative material not yet optimized at the industrial scale, was conducted together with the *Institut National des Sciences Appliquées de Lyon* (INSA), in which the *Laboratoire des Procédés et Matériaux Polymères* was working on the definition of a bio-based polymer (polybutylene succinate, PBS) using a pilot plant. In this research work, instruments available in the laboratory were utilized for the pilot production (a few kilograms of polymer pellet) of PBS, which will be produced at the industrial scale only in the future. In this case, different parameters of the pilot plant were monitored to forecast the environmental burden of PBS once it is produced using an optimized technology at the industrial scale. In this project, the concept of *ex-ante* LCA was adopted to forecast the optimized environmental performance based on the pilot-scale performance combined with the properties of the material.

The second work in which LCA was used, the definition of a methodology able to include uncertainty analysis and the capacity to use a LCT approach along the different phases of the building design process, was conducted in collaboration with the *Materials Systems Laboratory* (MSL). The context of this project was the development of innovative technologies by designers in the residential building sector. A chasm between the theory and practice of LCA was highlighted, particularly the fact that LCA is often applied at the end of the design process, excluding the possibility of making decisions at the earlier stages using environmental results as a metric of evaluation. Additionally, a quantification of uncertainty was often missing from the results, depriving the decision-making process of the necessary robustness. In this specific work, uncertainty analysis and the Probabilistic Underspecification approach (developed by MSL for a previous project on electronic devices) were used to define an innovative LCT approach for designers, providing the ability to obtain LCA results with associated uncertainty information in the early concept design phase.

Thanks to the experience gained at the MSL, some of the concepts of the uncertainty analysis were applied to the PBS project to refine the results and a strategy for future developments. Thanks to this fundamental update, the results are now available as probability distributions and not as single deterministic values.

The structure of this thesis begins with an introduction focused on the LCA methodology in service of materials and technologies, followed by the work performed at MSL (probabilistic underspecification for building assemblies and hybrid models obtained from probabilistic triage). The following two chapters are dedicated to the research on PBS, beginning with the evaluation of the environmental performance by means of LCA indicators using a cradle-to-gate approach, then an evaluation of uncertainty in the context of a multi-criteria material selection process (environmental performance and mechanical properties). In conclusion, final remarks and a discussion of the different approaches adopted and developed are provided.

1 INTRODUCTION AND LITERATURE REVIEW

In 1990, the Society of Environmental Toxicology and Chemistry (SETAC) coined the term Life Cycle Assessment to describe an approach that first came into being in the 1960s for a comparative efficiency analysis (energy and material consumption) of two or more systems (Baldo 2008). Later, the International Organization of Standardization (ISO) developed specific standards for the application of the methodology, which was considered one of the most important tools in the 1990s (Baumann and Tillman). These standards allow the methodology to be internationally recognized both within and outside of the scientific community. Nevertheless, a full-fledged LCA is still considered time-consuming and is characterized by high costs, which may represent a constraint for present and future sustainable development.

In this introduction, the framework of the methodology will be given as well as a description of the main issues that arose during its application. Then, an overview of the possible ways to streamline the analysis, forecast the results using different systems, and manage the uncertainty is provided.

1.1 ORIGINS AND USES

Life Cycle Assessment is a structured, comprehensive and standardized scientific approach, often used behind modern environmental policies and business actions related to sustainable development (ILCD Handbook - JRC 2010; ISO 14040 2010; ISO 14044 2010). In this context, the scientific community recognizes LCA as a relatively new (and developing) environmental management technique that has been having a very wide application since the mid-1980s (Rebitzer et al. 2004; Finnveden et al. 2009; Bieda 2014). This rise is also highlighted by the growing awareness of environmental issues by common people and internet users, as it is demonstrated by the exponentially increase of searches related to carbon footprint facts and statistics on web search engines (Michel et al. 2011).

Therefore LCA is broadly applied in practice (Finnveden et al. 2009) and LCA analysts consider LCA as a good tool to examine the environmental impacts of products, a quantitative way to estimate the life cycle resources and burdens, as well as a way to quantify alternatives in product systems (Cooper and Fava 2006). It is also considered by practitioners a powerful decision-making tool, especially for the market growth of innovative and environmentally responsible products. The market, indeed, has become more aware of the value of environmentally conscious materials selection and product development, as is evident in the proliferation of consumer-conscious “green” labels on products ranging from groceries to consumer electronics (Patanavanich 2011).

1.2 LIFE CYCLE ASSESSMENT FRAMEWORK

The increased awareness of the importance of environmental protection and the possible impacts associated with products, both manufactured and consumed, has increased interest in the development of methods to better understand and address these impacts. A most suitable technique being developed for this purpose is Life Cycle Assessment. According to ISO 14040 (ISO 14040 2010), LCA can assist in:

- identifying opportunities to improve the environmental performance of products at various points in their life cycle,
- informing decision-makers in industry, governmental or non-governmental organizations (e.g. for the purpose of strategic planning, priority setting, product or process design or redesign),
- selecting of relevant indicators of environmental performance, including measurement techniques,
- marketing (e.g. implementing an ecolabelling scheme, making an environmental claim, or producing an environmental product declaration).

LCA addresses the environmental aspects and potential environmental impacts (e.g. use of resources and the environmental consequences of substances release) throughout a product's life cycle from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal (i.e. cradle-to-grave). For practitioners of LCA, ISO 14044 (ISO 14044 2010) details the requirements for conducting an LCA study; as shown in Figure 1.1 there are four main phases:

- the goal and scope definition phase,
- the inventory analysis phase,
- the impact assessment phase,
- the interpretation phase.

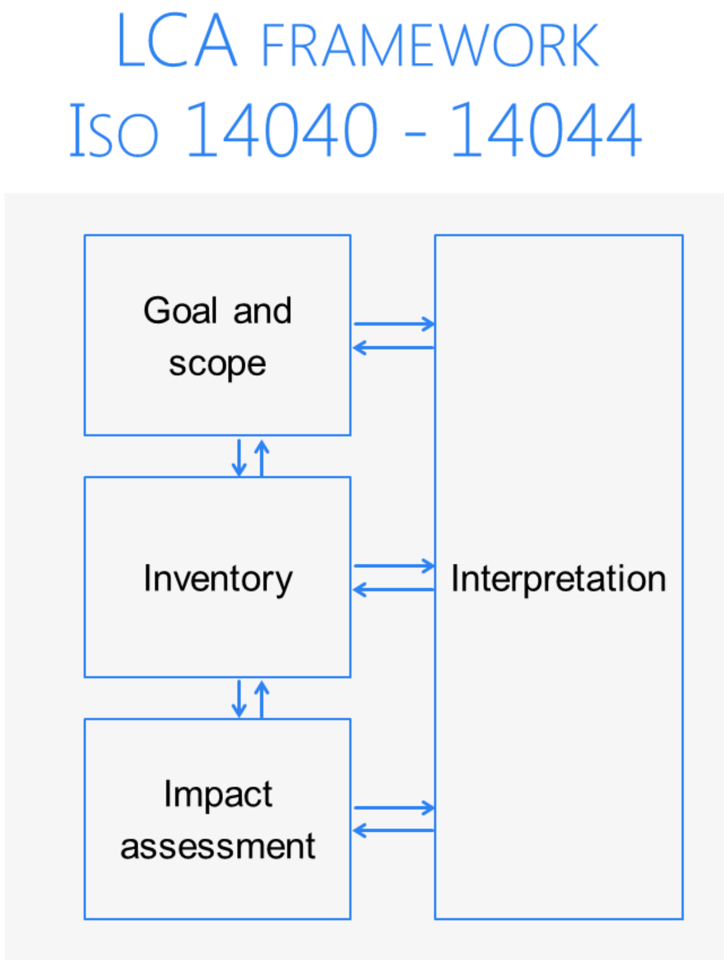

Figure 1.1 - LCA structure according to ISO 14040 and ISO 14044

- The Goal and Scope Definition, including the system boundary and level of detail, of an LCA depends on the subject and the intended use of the study. The depth and the breadth of LCA can differ considerably depending on the goal of a particular LCA;
- the Life Cycle Inventory analysis phase (LCI phase) is the second phase of LCA. It is an inventory of input/output data with regard to the system being studied. It involves collection of the data necessary to meet the goals of the defined study;
- the Life Cycle Impact Assessment phase (LCIA) is the third phase of the LCA. The purpose of LCIA is to provide additional information to help assess a product system’s LCI results so as to better understand their environmental significance;
- the Life Cycle Interpretation is the final phase of the LCA procedure, in which the results of an LCI or an LCIA, or both, are summarized and discussed as a basis for conclusions, recommendations and decision-making in accordance with the goal and scope definition.

LCA is one of several environmental management techniques (e.g. risk assessment, environmental performance evaluation, environmental auditing, and environmental impact assessment) and might not be the most appropriate technique to use in all situations. LCA typically does not address the economic or social aspects of a product, but the life cycle approach and methodologies described in these International Standards can be applied to these other aspects.

1.2.1 Mathematical approach

According to the General Guide for Life Cycle Assessment (ILCD Handbook - JRC 2010), LCI or LCA studies are often carried out using an iterative process, since during the life cycle inventory phase (and data collection) and during the subsequent impact assessment (and interpretation) more information becomes available, therefore initial scope settings will typically need to be refined or revised (Figure 1.2).

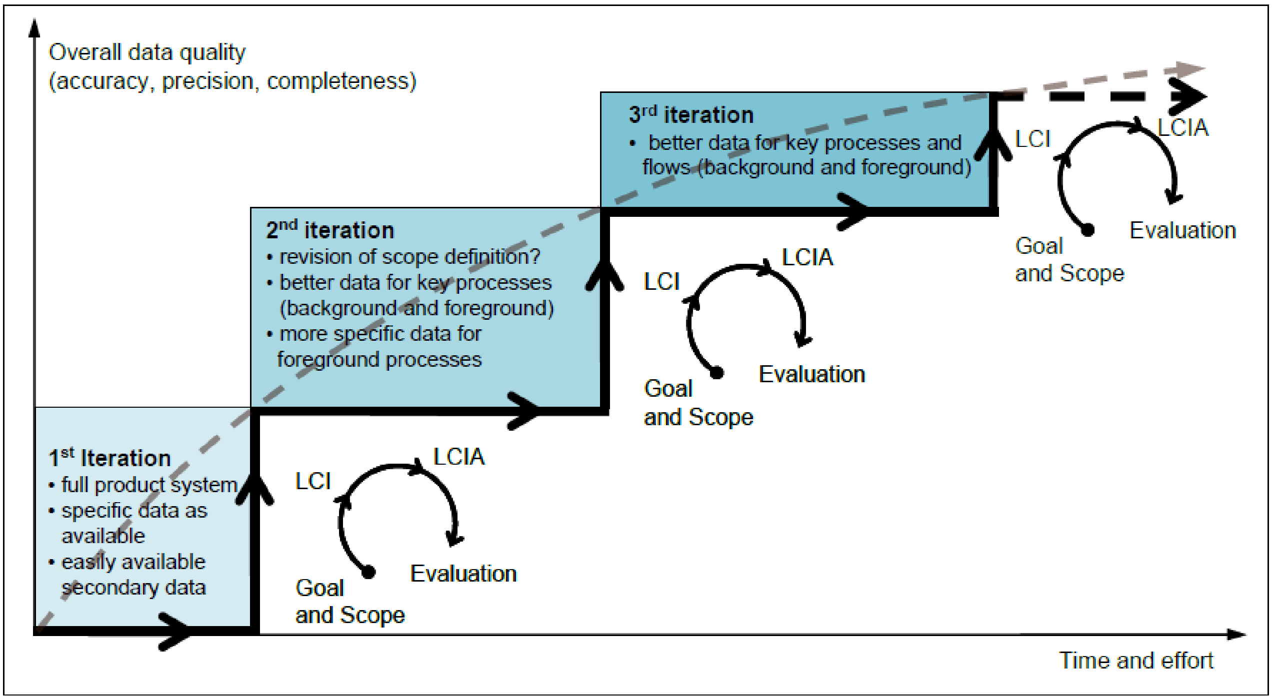

Figure 1.2 - Iterative nature of LCA (ILCD Handbook - JRC 2010)

The mathematical approach behind LCA allows to convert several environmental aspects (such as air and water emission, waste generation, consumption of energy and materials) into environmental impacts quantified and represented by few environmental indicators. In other words a potential impact on the natural environment, human health or the depletion of natural resources, caused by the events that occur between the technosphere and the ecosphere. The conversion of LCI data into LCIA results is obtained thanks to the use of *conversion factors* (also known as impact factors), available for each environmental aspect and for each environmental indicator. As an example, air emissions are considered (environmental aspects), such as carbon dioxide, methane and nitrous oxide (CO_2, CH_4, N_2O), well known to be greenhouse gases, it is possible to identify impact factors able to relate their potential environmental burden in terms of global warming potential (environmental impact). Global Warming (GW) is measured using CO_2 as reference substance, so other emissions are related to CO_2 using impact factors (25 kg CO_2 eq/kg CH_4 for methane, 298 kg CO_2 eq/kg N_2O for nitrous oxide). In this way, the potential effect on the environment of three different substances is summarized into a single (and simple) environmental indicator expressed as kg of CO_2 equivalent. In general, for a given environmental indicator, it is possible to describe the following equation, which is the basis of the mathematical approach:

$$Environmental\ Impact = \sum_{i=1}^{n} Quantity\ environmental\ aspect_i \cdot Impact\ Factor_i$$

1.2.2 Environmental indicators

The Life Cycle Impact Assessment phase helps to aggregate the inventory data in environmental indicators, in support of the interpretation phase. According to the General Guide for Life Cycle Assessment (ILCD Handbook - JRC 2010), LCIA methods exist at midpoint or endpoint level; both levels have advantages and disadvantages (Figure 1.3).

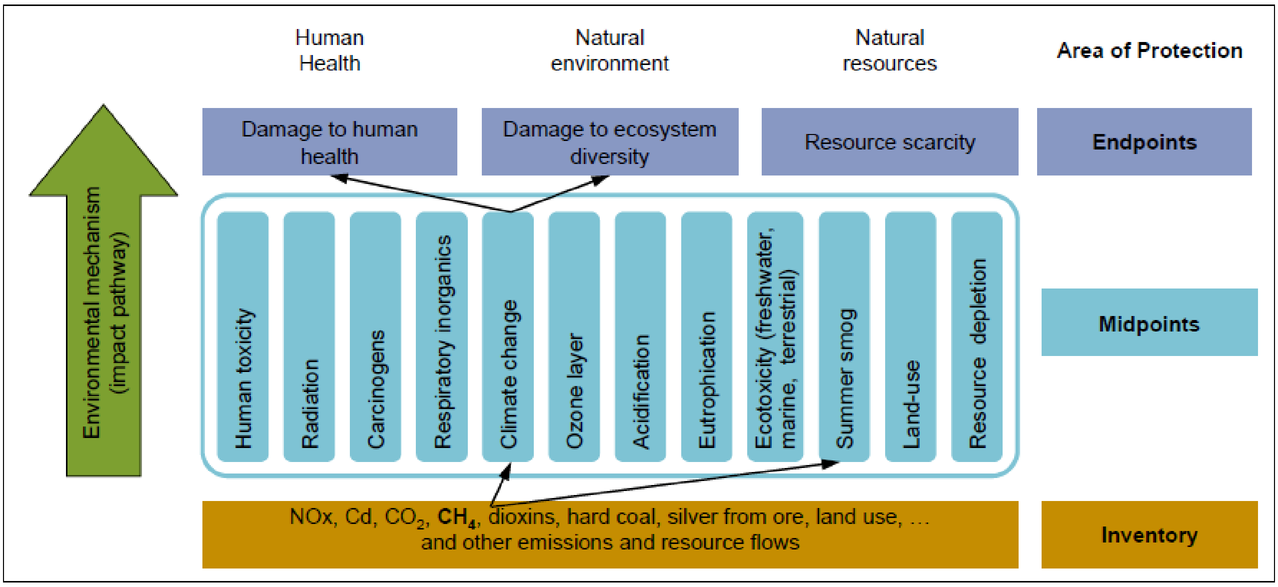

Figure 1.3 - Impact categories (midpoints and endpoints) of a Life Cycle Impact Assessment phase (ILCD Handbook - JRC 2010)

The following midpoint impact categories proved to be of high relevance during LCA studies and are currently broadly used for environmental product declarations. A description is provided hereinafter (www.leonardo-energy.org).

Global Warming (GW). Global Warming Potential is a measure of the effect on solar radiation (both direct or reflected) of a particular quantity of a substance over time relative to that of the same quantity of carbon dioxide. Therefore GW is an impact category that groups greenhouse gases (GHG) and calculate their total impact in terms of kg CO_2 equivalent, according to the IPCC (Intergovernmental Panel on Climate Change) reference document on Climate Change, in which the Global Warming Potential value for CO_2 is chosen as equivalence factor. Since Global Warming Potential depends on the time spent in the atmosphere by the gas, GW is calculated for the time horizon 100 years. Impact factors for different substances are evaluated combining climatic and chemical models able to covers two effects: the direct effect a substance has through the absorption of infrared radiation and the indirect chemical effects on overall radiation.

Cumulative Energy Demand (CED). Cumulative Energy Demand (or Gross Energy Requirement) calculates the total energy consumption of a specific system. It includes the primary energy demand, in other words the quantity of energy directly extracted from the hydrosphere, atmosphere or geosphere (natural gas, crude oil, coal, uranium, lignite, hydropower, wind power, solar energy and biomass). It is typically measured in MJ, using the Gross Calorific Value as reference for fuels. Indeed, for fossil fuels, biofuels and uranium, this would be the amount of resource withdrawn expressed in its energy equivalent (the energy content of the raw material identified by the Gross Calorific Value). For renewable resources, hydropower as an example, it would be based on the amount of energy that is gained from the change in the potential energy of the water (i.e. from the height difference). The energy content of the manufactured products is considered as feedstock energy.

Acidification (AP). The acidification of soils and waters occurs predominantly through the transformation of air pollutants into acids. This leads to a decrease in the pH-value of rainwater and fog from 5.6 to 4 and below. Sulphur dioxide and nitrogen oxide and their respective acids (H_2SO_4 und HNO_3) produce relevant contributions, therefore sulphur dioxide is the reference substance for this environmental indicator (acidification potential is given in sulphur dioxide equivalents, kg SO_2 equivalent.). The Institute of Environmental Sciences (CML) of Leiden University provided the impact factors for the mathematical algorithm. When analyzing acidification, it should be considered that although it is a global problem, the regional effects of acidification can vary.

Eutrophication (EP). it is the enrichment of nutrients in a given area, either aquatic or terrestrial. Air pollutants, waste water and fertilization in agriculture all contribute to eutrophication. The result in water is an accelerated algae growth, which prevents sunlight from reaching the lower depths. This leads to a decrease in photosynthesis and oxygen production, which is also needed for the decomposition of dead algae. Both effects cause a decreased oxygen concentration in the water, which can eventually lead to fish dying and to anaerobic decomposition (decomposition without the presence of oxygen). Hydrogen sulphide and methane are thereby produced and this can lead to the destruction of the eco-system. On eutrophicated soils, an increased susceptibility of plants to diseases and pests is often observed, as is a degradation of plant stability. If the nutrification level exceeds the amounts of nitrogen necessary for a maximum harvest, it can lead to an enrichment of nitrate and this effect can cause, by means of leaching, increased nitrate content in groundwater. The eutrophication potential is calculated in phosphate equivalents kg $PO_4{}^{3-}$ equivalent and impact factors for different substances are provided by the Institute of Environmental Sciences (CML) of Leiden University. As with acidification potential, it's important to remember that the effects of eutrophication potential differ regionally.

Photosmog (or simply Smog) creation (SM). Despite playing a protective role in the stratosphere, at ground-level ozone is classified as a damaging trace gas. Photochemical ozone creation in the troposphere, also known as photosmog, is a cause of damage for vegetation and materials. Moreover, high concentrations of ozone are toxic to humans. Radiation from the sun and the presence of nitrogen oxides and hydrocarbons incur chemical reactions that produce aggressive reaction products, one of which is ozone (O_3). Hydrocarbon emissions occur from incomplete combustion, in conjunction with petrol (storage, turnover, refueling etc.) or from solvents. High concentrations of ozone arise when the temperature is high, humidity is low, when air is relatively static and when there are high concentrations of hydrocarbons. Because carbon monoxide (CO, mostly emitted from vehicles) reduces the accumulated ozone to CO_2 and oxygen, high concentrations of ozone do not often occur near hydrocarbon emission sources. Higher ozone concentrations more commonly arise in areas of clean air, such as forests, where there is less CO. In LCA, photochemical ozone creation potential (POCP) or photosmog creation (SM) is referred to ethylene-equivalents (kg C_2H_4 equivalent.) and impact factors for different substances are again provided by the Institute of Environmental Sciences (CML) of Leiden University. When analyzing, it's important to remember that the actual ozone concentration is strongly influenced by the weather and by the characteristics of the local conditions.

Many of these impact categories are grouped in assessment algorithms. TRACI, for example, is a midpoint oriented life cycle impact assessment methodology developed by the U.S. Environmental Protection Agency and includes impact categories like global warming, acidification, eutrophication (measured as kg N eq), tropospheric ozone (smog) formation (measured as kg O_3 eq), human health criteria-related effects (respiratory effects) (Bare et al. 2006; Bare et al. 2012; SimaPro 2013).

1.2.3 Environmental Product Declarations

An environmental declaration is defined as quantified environmental data for a product with pre-set categories of parameters based on the ISO 14040 series of standards, but not excluding additional environmental information (ISO 14025 2006). An environmental declaration is created and registered in the framework of a type III environmental declarations program, such as the International EPD® System, which is a system of verification and registration of EPD®s based on a library of existing EPD®s and Product Category Rules (PCRs), in accordance with ISO 14025 (Environdec).

An Environmental Product Declaration (EPD) can be classified as an ISO Type III environmental labelling system (quantified environmental life cycle product information). Other possible environmental labels can be grouped in ISO Type I environmental labels (voluntary, multiple-criteria-based, third party verified labels indicating overall environmental desirability of a product) and ISO Type II environmental labels (self-declared environmental claims). The most important features of a Type III environmental label are the non-selective procedure (environmental excellence has not to be demonstrated and technically all products or services can access the system) and the use of environmental indicators to measure and quantify the environmental performance of a system. In Figure 1.4, Figure 1.5 and Figure 1.6 it is possible to appreciate the volume of EPDs produced and published on the International EPD® System platform. Charts detail the category types (foods and construction products are the main contributors), growth rate from 2008 and finally a breakdown of the registered declaration per country, with a leading role for Italy and Sweden.

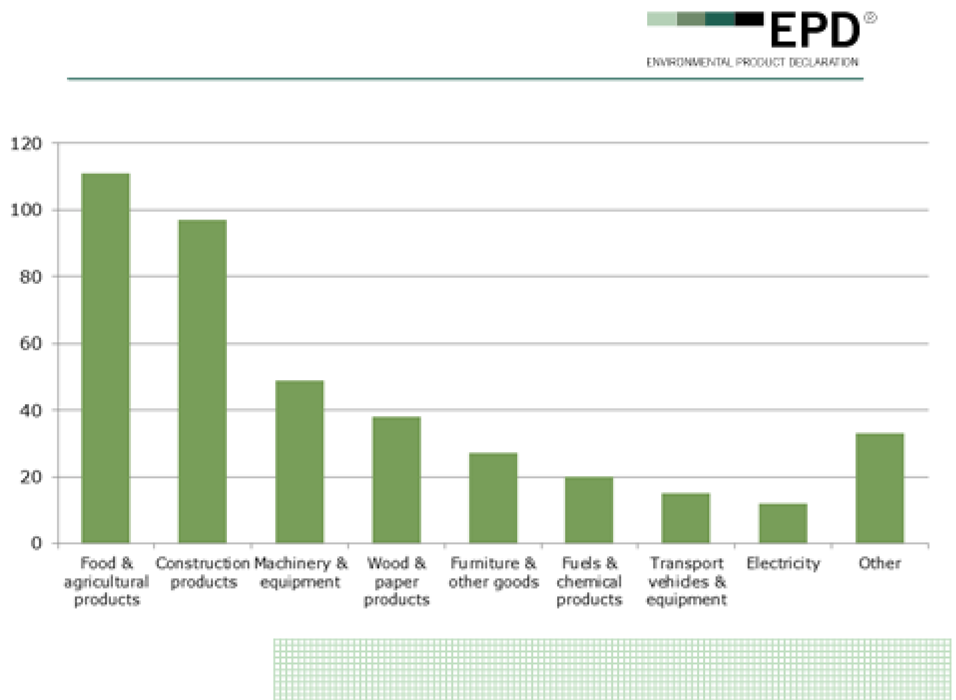

Figure 1.4 - Number of EPDs registered by category (courtesy of The International EPD® System)

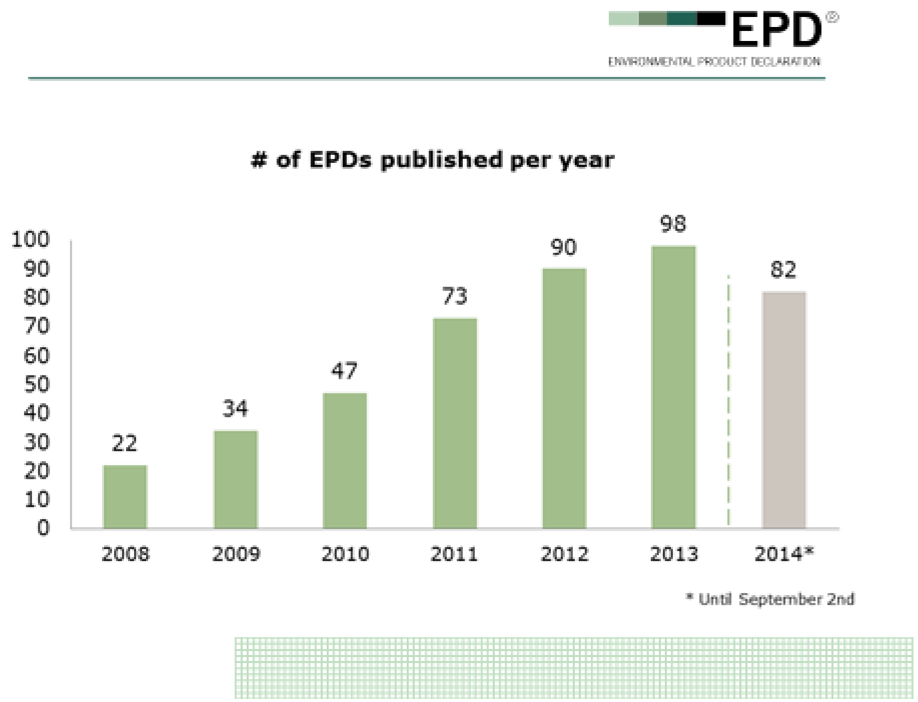

Figure 1.5 - Number of EPDs published per year (courtesy of The International EPD® System)

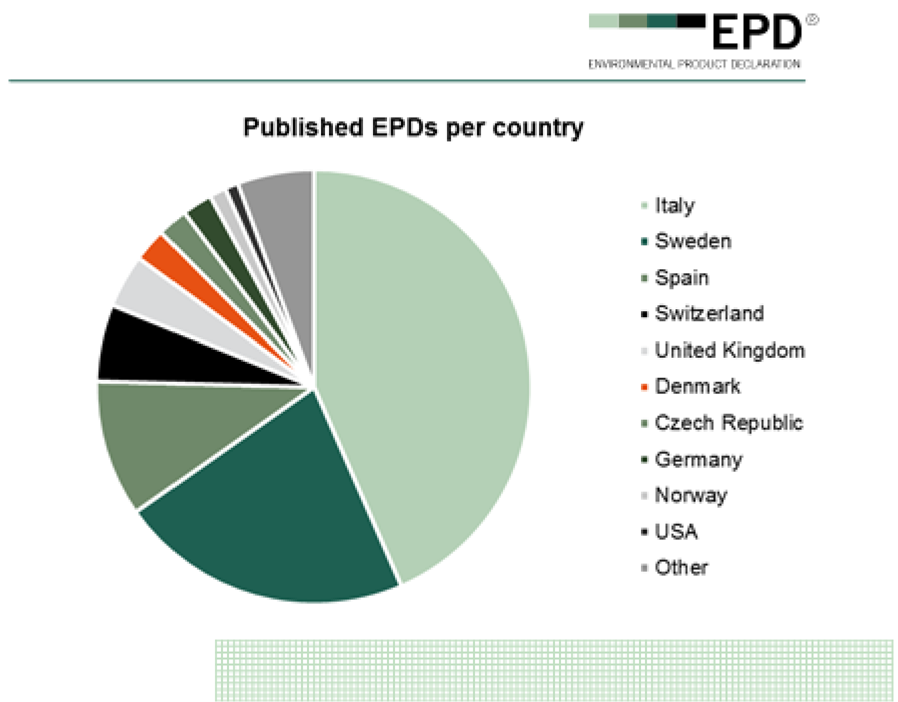

Figure 1.6 - Published EPDs per country (courtesy of The International EPD® System)

1.2.4 Issues in LCA application

LCA is a relatively new methodology, so characterized by strengths and weaknesses (Finnveden et al. 2009). Based on a survey (Cooper and Fava 2006) of LCA practitioners and designers, the use of the methodology is considered "limited" and not massively applied to more products and processes because of:

- Time and resources requirements for the collection of data;
- complexity of the LCA method;
- lack of clarity as to the relative benefits compared to the costs of conducting the LCA studies;
- lack of apparent downstream interest or demand.

The first point highlights how LCA is a resource intensive methodology: the main cost driver is the large amount of information needed to identify the overall life cycle of a system, given that a full-fledged LCA requires all of the inputs and outputs for all phases of the considered system boundaries. Conducting the LCI analysis may imply the collection of complete information even for the simplest commodity and may require significant time and resources (Patanavanich 2011). Moreover existing data gaps, either in the data collection and in the modeling phase, pose a frequent challenge, motivating the need for robust streamlining approaches (Reis 2013). An effective and efficient approach to LCA is of fundamental importance for the sustainable development, especially when limited information are available about the product's supply chain and life cycle (Chen and Wai-Kit 2003).

Reap et al. (2008) published results of a survey of unresolved problems in life cycle assessment, according to the point of view of practitioners. Multiple problems occur in each phase of the LCA framework, but data availability and quality are identified by practitioners as critical problems affecting all four phases. Therefore LCA suffers from problems that degrade accuracy and increase uncertainty of assessment results: problems encountered during goal and scope definition arise from decisions about inclusion and exclusion; the exclusion of economic and social impacts in LCA sets fundamental limits on the comprehensiveness of the tool; the choice of alternative scenarios influences decisions in the interpretation phase; inventory analysis problems include definitions of allocation procedures, flows, transformations and criteria used to identify and eliminate unimportant resource; setting arbitrary time horizons skews results in favor of short- or long-term impacts and aggregation is considered the principal problem occurring during the interpretation phase (Reap et al. 2008).

Another recent research was developed by Finnveden et al. with more objectiveness, excluding personal problems and issues, focusing on the mathematical framework and highlighting recent developments in relation to some of the strengths and weaknesses of the tool (Finnveden et al. 2009). First of all LCA is a data intensive methodology, therefore limited data or lack of information can affect the conclusions that can be drawn from a specific study; this issue may be solved primarily with better databases and a better experience by the life cycle analyst, but this requires a previous knowledge able to tell us where to focus our efforts. Furthermore, LCA aims at providing a comprehensive view of environmental impacts, but not all types of impacts are equally well covered; for example, methods for the Impact Assessment of land use, including impacts on biodiversity, and resource aspects, including freshwater resources, are problematic and need to be improved. LCA involves several methodological choices which are uncertain and may potentially influence the results; examples include allocation methods, time limits for the Inventory Analysis and questions related to system boundaries. Finally, different types of uncertainties characterize the use of the methodology and this represents an important issue; a special type of uncertainty is related to lack of knowledge on the actual system to be studied; this is the case, for example, for future systems and technologies, since the future is intrinsically uncertain (Finnveden et al. 2009).

1.3 Uncertainty analysis in LCA

According to the definition provided by the ISO Guide to the Expression of Uncertainty in Measurement, uncertainty is a parameter associated with the result of a measurement (for example the standard deviation) that characterizes the dispersion of the values that could reasonably be attributed to the quantity intended to be measured (ISO 2008). Thus, uncertainty is linked to measured values that cannot be exactly repeated in other measurements (due to errors) and are generally represented by probability distributions.

Concerning the LCA methodology, the U.S. Environmental Protection Agency listed three main sources of uncertainty and variability. Uncertainty in observed or measured values used in a model is called parameter uncertainty; it is almost always considered in LCA studies with data uncertainty regarding process inputs, environmental discharges and technology characteristics. Scenario uncertainty relates to, for example, the normative choices in constructing scenarios and the inherent variability in scenario characteristics given various geographical locations or situations. Models themselves may add uncertainty and there may be variability between models because of the structure and mathematical relationships in the models (Lloyd and Ries 2008). The same three types of uncertainty were defined by Huijbregts et al. (2003).

Therefore, even though the LCA methodology has developed and matured, a remaining problem of LCA is the existence of uncertainties and variations in data. This represents a limitation for a clear understanding and interpretation of LCA results. LCA studies, to be robust and credible, should communicate the reliability of their results in terms of uncertainty based on an assessment of the data quality of the information used (Weidema 2000; Bieda 2014). This means that a single deterministic LCA result might not be enough for a clear understanding and interpretation of the environmental performance of a system. A probabilistic distribution of LCA results is, on the other hand, a robust way to represent the uncertainty and variation of the data in a data collection and LCI analysis (Sonnemann et al. 2003). Policy makers and decision makers need high credibility form methodologies like LCA, since the outcomes of such studies can significantly reflect on the financial stability (de Koning et al. 2009).

Several studies evaluated the role of different types of uncertainty and from a literature review it emerged that all three types of uncertainty can be important, but the most frequently addressed type is the parameter uncertainty. Several approaches for conducting LCA under uncertainty have been proposed and implemented: stochastic modeling, scenario modeling, fuzzy data sets, interval calculations, analytical uncertainty propagation and Bayesian statistics are the most important. Monte Carlo simulation and fuzzy set theory have been applied in a limited number of LCA studies, but these approaches are well understood and are generally accepted in quantitative decision analysis. However, reliable outcomes cannot be 100% guaranteed (Lloyd and Ries 2008).

1.3.1 Perturbation theory

Heijungs and Suh (2002) discussed the theory of the computational structure of LCA, with an emphasis on uncertainty characterization through the perturbation theory. In their book, the authors note that this theory is of particular significance and can be used for a number of interesting subjects in LCA, including the propagation of unit processes uncertainties into uncertainties of scaling factors or environmental results.

In general terms, an LCA model is based on physical quantities *q*, i.e. parameters, for which a series of impact factors *F* can be identified, such as global warming potential, eutrophication potential, acidification potential, etc. The impact assessment can provide deterministic results *EI* using the following relationship (1.1):

$$EI = \sum_{i=1}^{n} q_i \cdot F_i \tag{1.1}$$

Where *n* represents the number of physical quantities/elements of the LCA model.

The perturbation theory studies the influence of perturbations of coefficients of equation on the solutions to those equations. If an LCA dataset realized using several parameters is considered (material and energy flows, products, emissions and waste), uncertainty is associated with each parameter thanks to the description of the probability function and the standard deviation.

Therefore the single deterministic result in this approach becomes a vector of results that originates the perturbed matrix, a function of the original value plus a perturbation term (δ):

$$EI' = EI + \delta EI \tag{1.2}$$

Because the parameters of the LCA model are characterized by uncertainty as well, perturbed parameters are calculated as follows:

$$q' = q + \delta q \tag{1.3}$$

In detail, the entire simulation is run several times, in order to have a significant number of trials. In the end, each parameter of the LCA dataset is characterized by a distribution of results, which are then aggregated to the others in order to have the total probabilistic distribution.

1.3.2 Monte Carlo simulation

One of the main challenges of LCA is to measure and to quantify uncertainty related to results. To achieve this goal many tools use Monte Carlo analysis as a stochastic simulation model. Monte Carlo analysis is a numerical way to process uncertainty data and establish an uncertainty range in the calculated results (Simapro 2013). This method generates parameter values with random variables drawn from probability density functions (LaGrega et al. 2010), typically provided by LCA databases like EcoInvent[1]. Within these databases, information about uncertainty at the LCI level are available and can be processed by means of a probability function (e.g., lognormal distribution) and a measure of uncertainty (e.g., standard deviation) for each single parameter of an LCA dataset.

During a Monte Carlo simulation, a computer takes a random variable for each value within the uncertainty range specified by the user and recalculates the results. The next calculation (also called *iteration*) is repeated by taking different samples within the uncertainty range. After repeating the procedure for instance 1000 iterations, 1000 different answers can be obtained and they form probability density function (results distribution) (Simapro 2013).

Standard distribution types, such as range, triangular, normal and lognormal distribution, can represent uncertainty:

- range distribution (minimum and maximum values are needed);
- triangular distribution (minimum, maximum and the median value are needed);
- normal distribution (standard deviation and median value are needed);
- lognormal distribution (standard deviation and median are needed, Figure 1.7).

Several reasons justify the use of lognormal distribution as predominant probability function in such databases; first of all, lognormal distribution is frequently observed in real life populations (Koch 1966), it is

[1] http://www.ecoinvent.ch/

representative of many LCA input parameters (Huijbregts et al. 2003) and the highest amount of parameters for real life populations are always positive (Weidema et al. 2013).

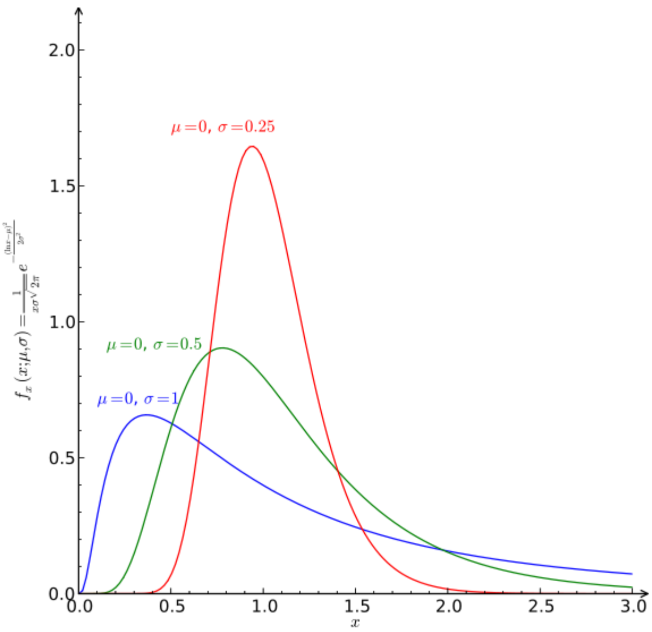

Figure 1.7 - Lognormal density functions with identical location parameter (μ) and different scale parameters (σ). Source: Wikipedia.

In the present thesis, Monte Carlo method was used to process the uncertainty data for all of the assessments. This way, for each parameter, there is not just one value representative of the impact, but a range of data points (domain of possible inputs) defined by a probability distribution and standard deviation. Monte Carlo simulation randomly generates inputs from probability density functions over the domain and performs a deterministic computation on generated inputs. 1000 iterations were used to guarantee reproducibility in results (Steen 1997). Finally, results are aggregated and represented by means of boxplot charts (an example in Figure 1.8).

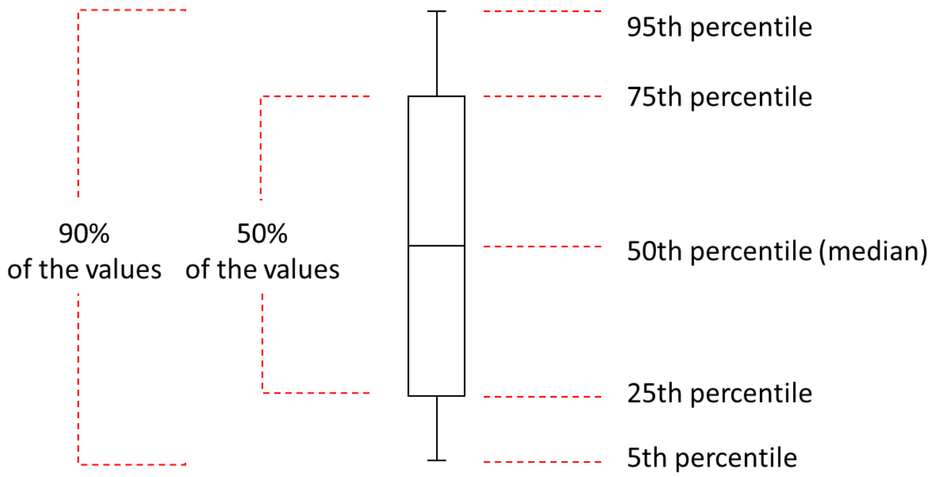

Figure 1.8 - Boxplot chart example. Definition of a probability distribution by means of 5th, 25th, 50th, 75th and 95th percentiles.

1.3.3 Pedigree matrix

Life cycle models are characterized by uncertainty. PRé Consultants, developer of the LCA software package SimaPro, distinguishes three main types of uncertainty for models built in its tool:

- variation in the data;
- correctness (representativeness) of the model;
- incompleteness of the model.

Variation in the data consists of the parameter uncertainty described in chapter 1.3 and can be described, as stated in section 1.3.2 by a probability distribution (Simapro 2013). In the case of ex-novo datasets, LCA practitioners directly define the basic (parameter) uncertainty, through the calculation of the probability distribution and the standard deviation for each parameter, provided that sample data of measurements are available. Furthermore, additional uncertainties from data quality indicators are typically added; these additional uncertainties are based on the pedigree matrix approach proposed by Weidema (Weidema and Wesnaes 1996; Weidema 1998).

EcoInvent uses the pedigree matrix to estimate geometric standard deviations. For each dataset, each data point is assessed based on six criteria plus the basic uncertainty factor (which depends on the type of data). The 95% confidence interval or the squared geometric standard deviation σ is calculated using equation (1.4):

$$\sigma^2 = \sum_{i=1}^{6} \sigma_i^2 \tag{1.4}$$

The factors σ_1 to σ_5 refer to the scores obtainable in reliability (1), completeness (2), temporal correlation (3), geographical correlation (4) and further technology (5) of the pedigree matrix (see Appendix A - Pedigree matrix). The factor σ_6 refers to the basic uncertainty factor (see Appendix A) (Simapro 2013). In the present work, the pedigree matrix was used to process uncertainty for each data point.

1.4 STREAMLINED LCA APPROACHES

As already stated in the previous chapters, nowadays technological progress is closely connected with sustainable development. This means that innovations (for example a new generation of hybrid engines or a new electronic device for telecommunication or even innovative techniques to build a house, for instance) are now studied and designed with particular attention to environmental performance, in other words the future impact on natural ecosystems. This kind of human activity impact assessment is the result of the LCT approach and one way to evaluate the environmental sustainability of a system is to use the LCA methodology, whose principal aim is to specify the environmental consequences of products and services from cradle to grave (ACADEMY 2008; Finnveden et al. 2009; Curran 2013). However, a full-fledged LCA study may be complex, expensive and time consuming (Hochschorner 2003; Schulz et al. 2012), therefore the practice of streamlining LCA began to be studied and developed using different approaches (Baumann and Tillman; Pesonen and Horn 2012).

Streamlined LCA can be achieved in several ways. From a literature review it is possible to classify them into three main groups: (1) methods that limit the scope of the analysis, excluding minor activities or phases characterized by negligible environmental burden (Bala et al. 2010; Schulz et al. 2012); (2) methods that use qualitative or semi-quantitative information and business planning approaches (Hochschorner 2003), (Pesonen and Horn 2012); (3) methods that promote the use of specific impact categories and qualitative results to facilitate interpretation (Kloepffer 2008; Finkbeiner et al. 2010).

A number of life cycle approaches exists: qualitative LCAs, simplified LCAs, life cycle influence matrices, LCA-derived proxies, hot spot analysis, combination tools, sustainability matrices, etc. An exhaustive literature review on these techniques has been carried out by Pesonen and Horn (2012). The strengths and weaknesses of these different approaches are presented in Appendix C - Streamlined LCA approaches. Moreover, in their study they recall the three basic levels of LCA (Wenzel 1998):

- a full-fledged (full-scale) LCA, quantitative and including new data inventory;
- a screening LCA, quantitative and using readily available data or semiquantitative information;
- a matrix LCA, qualitative or semiquantitative.

Pesonen and Horn (2012) stated that both screening and matric LCAs are the only levels seen as streamlined approaches. In the first approach, quantitative data is used even though there is no need for new inventory calculation, while in the latter, qualitative and semiquantitative information is used. However, they observed that it is not the ultimate ambition of streamlined approaches to substitute a full-scale assessment. Rather, their goal is to show how simplified model, opportunely adapted, can be useful in providing measures of environmental impact or a quick overview of a product's environmental profile.

From this recent literature review it is clear that a streamlined LCA approach is considered as a tool that must be as simple as possible, but this can introduce some criticality in the algorithm. In general, the scientific community is not considering the possibility to develop a robust methodology that can be used in lieu of a full-scale LCA.

As there are obviously many sources of uncertainty in measures and in the methodology itself, there has arisen a need to systematically incorporate uncertainty into the assessment. Keeping in mind that a streamlined LCA approach can increase the uncertainty, it would be appropriate to try to deal with this issue in the streamlined methods as well. An approach is required to manage uncertainty with transparency, fairness, and competence (Pesonen and Horn 2012).

1.4.1 Requirements for a comprehensive approach

A streamlined LCA approach should support the design process and reduce cost and time for LCA implementation. Moreover, it should be characterized by a reduction of efforts associated with the bill of activities characterization (BOA) as well as the burden in characterizing the LCI associated with these activities (Olivetti et al. 2013). Many tools have been proposed (Graedel et al. 1995; Chen and Wai-Kit 2003; Hochschorner 2003) but only few authors have explored the relative strengths and weaknesses of these approaches (Olivetti et al. 2013), like the system boundary assumptions, cut off criteria and data collection procedures through the use of less accurate data or surrogate processes (Hunt et al. 1998).

However, a comprehensive approach should provide quantitative results, achieved without cutting off any part of the system life cycle; moreover, it should be developed with an uncertainty analysis of results, in order to be applicable in different phases of the design process. When LCA is used as a decision-making tool, uncertainty is a crucial issue (Huijbregts 2001; Geisler et al. 2005; Lloyd and Ries 2008) and the deterministic environmental results obtained by an ex-ante analysis (a preventive analysis conducted on concept design or lab-scale productions) cannot be compared with the ones obtained by an ex-post study (an LCA applied to a fully developed system). An uncertainty analysis of results is strongly recommended to support decisions with robustness and reliability in computational models. Even though LCA practitioners often fail to properly address the issue of uncertainty quantification in their reports (Ross et al. 2002), understanding of the uncertainty contributions of each of the LCA components is crucial and will facilitates the improvement of the credibility of LCA (Hung and Ma 2008).

1.5 LCA AND SUSTAINABILITY PROTOCOLS FOR BUILDINGS

The increased awareness of environmental sustainability in the construction sector has resulted in the growth of various building assessment frameworks and rating sustainability tools (Schwartz and Raslan 2013), widely discussed in the "Guide to Building Life Cycle Assessment in Practice" written for The American Institute of Architects (AIA) (Bayer et al. 2010). The Building for Environmental and Economic Sustainability (Bees®) is an example of building product tool that compares different building products. The Athena Institute developed the Athena Impact Estimator for Buildings®, a building LCA tool in which, however, the impact of the operational use phase cannot be calculated. The Economic Input Output – LCA (EIO-LCA) is an economic input-output LCA-based free tool developed by Carnegie Mellon University, that evaluates the embodied phase, in other words the "cradle-to-gate" phases of the building's life cycle: materials extraction and manufacturing, construction, maintenance, repairs and transportation.

From the building sector perspective, many are the tools that proved to be internationally helpful for the evaluation of the environmental impact of buildings. Life cycle simulation tools such as EQUER, the Australian LCAid, Eco-Quantum for residential buildings, Envest, Team, as well as other commercial tools are typically used by LCA specialists (SimaPro, GaBi, The Boustead Model, Umberto, etc.) (Bayer et al. 2010).

Furthermore, numerous countries have developed green building programs aimed at promoting more sustainable buildings, such as LEED (Leadership in Energy and Environmental Design), a rating system developed by the US Green Building Council (Newsham et al. 2009). The use of these programs aims to reduce the environmental burden of a new building, even though this idea drew criticism and opposed opinions. Newsham et al. elaborated data about 100 LEED-certified commercial and institutional buildings and estimated that LEED buildings used 18–39% less energy per floor area than their conventional counterparts. Further, the measured energy performance of LEED buildings had little correlation with certification level of the building, or with the number of energy credits achieved by the building at design time (Newsham et al. 2009). Scofield directly replied to that research explaining that conclusions hang on a particular definition of the mean energy intensity of a collection of buildings. That definition is not related to the total energy used by those buildings. Site energy considered by Newsham et al. does not account for the energy consumed off-site in generating and delivering electric energy to the building, whose inclusion is crucial for understanding greenhouse gas emission associated with building operation (Scofield 2009).

1.5.1 Building design process

Even though theoretically LCA can be used in different stages of the design process, actually the application is still challenging. Full-fledged LCA studies are typically carried out during the last stage of the design process, because that is the moment in which a complete bill of materials or bill of activities is available for a robust inventory.

AIA identifies three typical stages of the architectural design process to address the problem of the level of detail needed by LCA to be applied (Bayer et al. 2010): (1) Pre-Design Stage, in which LCA can define the environmental targets of a specific project and simplify decision-making regarding the different options available for building features, in order to have basic trade-offs between impacts from the manufacturing and operational phases; (2) Schematic Design Stage, which is a more detailed level and choices regarding the use of specific building products (for example, assemblies or materials) can be made using LCA; (3) Design Development Stage, in which detailed design drawings are produced by architects and engineers for envelope and structure, heating and cooling plant, services and installation (Bayer et al. 2010), (AIA 1995).

Moreover, other reasons relegate the application of the methodology to LCA practitioners and specialists only. Researchers of the Massachusetts Institute of Technology conducted a survey asking architects and engineers from the construction sector their thought and feedback about LCA. The following critical features emerged: the complexity of the computational model, the complexity of data collection for inventory analysis, the need of expensive and sometimes cumbersome tools and the experience and skills required to assess the availability and completeness of data in LCA databases.

Eventually, the use of LCA tools by building design professionals is still uncommon. Even if the inventory analysis data have already been collected, tabulated and indexed, the time consuming issue associated with the methodology still exists and discourages designers because of the iterative process (Malin 2005).

1.5.2 Literature review

Following an exhaustive review of the construction sector literature, it is possible to highlight that there is a large production concerning the use of the LCA methodology for the evaluation of the overall environmental efficiency of buildings (Ghattas et al. 2013). According to this literature review, even if the operational energy consumption generally decreases thanks to improved energy efficiency, the so called embodied phase can increase because of the additional materials required for energy efficiency systems (Verbeeck and Hens 2010; Cuéllar-Franca and Azapagic 2012). Since the building codes are becoming more stringent, environmental awareness is increasing and demand for energy efficient buildings is increasing as well. As a result, it is becoming more relevant to consider the embodied phase as part of building codes and standards, analyzing possibilities for improvement and providing guidelines for materials selection in the Ecodesign of new buildings and rehabilitation of existing buildings (Zabalza Bribián et al. 2011).

The literature review focused on the LCA technical aspects demonstrating how there is no common methodology able to address all of the main building features, like geometry, lifetime and geographic location. Several works adopted the overall “standard” (typical for a specific region) building as functional unit, considering different floor areas and different climate regions (Mithraratne and Vale 2004; Hacker et al. 2008; Monahan and Powell 2011; Utama et al. 2012; Ihm and Krarti 2012). Other works used various segments of the building as functional unit (Blengini 2009; Bolin and Smith 2011; Allacker 2012), others a normalization with other parameters, using the unit of mass (1 kg) of materials for the construction (Zabalza Bribián et al. 2009) or the single building inhabitant (Heinonen et al. 2012). The building lifetime is another key parameter and in several works is included in the range 25-100 years. Longer term life cycle includes significant renovation activities (Börjesson and Gustavsson 2000), while shorter lifetimes are conceived in order to make results relevant in terms of meeting climate change mitigation goals set for the next few decades (Säynäjoki et al. 2012); in a recent work, Aktas et al. calculated the average residential building lifetime to be 61 years with a standard deviation of 25 years, based on the 2009 American Housing Survey (Aktas and Bilec 2011).

The system boundary definition may represent another point of discussion; Optis highlighted the lack of information for different research works, estimating that 60% of studies did not explicitly state which life cycle stages are included and 85% of the same set of studies did not identify the unit processes (e.g. materials) included within the boundaries (Optis and Wild 2010). Some of the studies excluded parts of the life cycle, for example the end of life, because judged negligible or less important (Gustavsson and Joelsson 2010; Monahan and Powell 2011). Furthermore, there is limited research on the renovation of existing housing with energy efficiency measures.

Another aspect that was not adequately considered in most publications is the quantification of uncertainty in results. The lack of a common LCA framework as well as the uncertainty associated with local primary data give a key role to the uncertainty analysis.

1.6 Ex-ante LCA approaches

Although results of conventional LCAs are accurate and acceptable, conceptual design stages are often characterized by incomplete information, thus making this method infeasible for use (Yang and Chen 2012). Indeed, the fast pace of technological progress and the increasing pressure on natural ecosystems put forward the urgent need for the assessment of the human activities impact, especially in the early stage of development (Roes and Patel 2011; Shields et al. 2011; Basbagill et al. 2013). In particular, the possibility to estimate the potential impact that a new product could have on the environment, ahead of its adoption, is of fundamental importance during the design phase (Thackara 2005). Currently, LCA is internationally considered the standard in environmental impact assessment and represents a scientific and structured methodology (Roes et al. 2009; Finnveden et al. 2009; Curran 2013), but in order to perform such analysis, a complete and deep understanding of the overall life cycle of a product system is required. In case of an innovative material that has to be analyzed with LCA, this condition can be satisfied once the material itself has been fully developed, produced, optimized and introduced onto the market. On the other hand, as already said, adequate information to perform an LCA study is often unavailable at the early design stage (Shields et al. 2011). Furthermore, when LCA is used as a supporting tool in decision making, it is argued that an expansion of the standardize framework is required by implementing other approaches and methodologies (Jeswani et al. 2010).

As far as early stage impact assessment (ex-ante LCA) of chemical processes is concerned, several methods have been proposed (Sugiyama et al. 2008; Bumann et al. 2010; Patel et al. 2012). Since the available information is limited at early stage, most of these methods are qualitative and not readily useful for a proper selection among alternative options. In particular, when comparing new materials at an early stage of development with industrially optimized ones, a production scale issue arises (Curran 2013). In fact, the production at lab/pilot scale cannot be directly compared to industrial systems, mainly due to the large discrepancy in the yield of the processes involved. Furthermore, those methods are commonly referred to bulk chemicals production processes (with a gate-to-gate horizon), but not to polymeric materials synthesis, and require detailed data about the reactions involved (Bumann et al. 2010).

1.7 Multi-criteria analysis

Since the importance of the anthropogenic impact on the environment has reached wide public awareness, the demand for sustainable products and services is continuously increasing (Maxwell and van der Vorst 2003; European Bioplastics 2013). In this context, Environmentally Conscious Design (ECD) and Ecodesign principles have gained relevance (Huang et al. 2009; Huang et al. 2010; Toso et al. 2012) and a series of tools and good practices for a sustainable approach to design have been developed since the 1990s (Zhang et al. 1997). Thackara (2005) estimated that about 80% of the environmental impact of products and services is determined at the design stage. Decisions taken in this early phase of a product/service life cycle will determine how it will be manufactured and delivered, how it will be used and how it will be disposed.

In this regard, the materials selection is one of the most crucial choices that a designer has to cope with. The selection process of an innovative material, to be used in place of another, is mainly based on the intrinsic properties of the material itself such as mechanical characteristics, thermal and electrical properties, cost, etc. However, a proper comparison in a change-oriented perspective should take into account both these properties and the environmental performance of the material. Nevertheless, since the LCA methodology presents some limitations, a need to expand the ISO LCA framework emerged. A more useful support to the decision-making process can be reached through the integration and connection with other concepts and methods (Jeswani et al. 2010; Curran 2013).

Multi-criteria analysis (MCA) is a systematic approach that demonstrated significant reliability in dealing with complex design issues. MCA is becoming a widely employed methodology in the energy and environmental sectors since the decision-making process has to include and assess a range of technological, economic, social, environmental, risk, financial, quality, and reliability considerations. By using MCA tools, a decision-maker has the ability to set its own objectives, as well as the significance of each in order to assess the effectiveness of different alternatives (Kylili et al. 2014).

1.7.1 Multi-criteria materials selection

The multi-criteria materials selection methodology used for the elaborations in chapter 5, is grounded in the approach developed by Prof. Ashby (2000). This methodology aims at comparing different materials on the basis of more than one property, i.e., considering at the same time mechanical performances, thermal properties, optical properties, cost, etc. This method is based on the identification of proper *material indices*, defined combining solid mechanics and materials science. These indices result from considerations about the geometry of the component and the stress conditions. Each index combines a defined set of properties (e.g. density, Young modulus, tensile strength, environmental impacts, etc.) and is used to compare alternative materials for a specific application, targeting the maximization of the required performance. To carry out such a comparison, material indices are graphically represented with Ashby plots (also known as bubble diagrams). On these diagrams a material property, or a combination of properties, is plotted as a function of another: each material is represented by a bubble localized within the area of the map (Ashby 2000). The mutual position of the bubbles mirrors how each material performs with respect to the others in the specific considered application.

1.7.2 Material indices and Ashby plots

In order to identify the most suitable *material indices* to be considered, an adequate formulation of the engineering problem to solve is necessary. In particular, the design process of a component must take into account 1) the function that the component has to fulfill and 2) the requirements and constraints to be met. Furthermore, a designer usually sets one or more objectives: e.g. minimizing the cost, reducing the mass of the component, lowering the environmental impact or a combination of thereof (Ashby 2010).

The performance of a component can be quantified by means of a *performance parameter* (P) that is mathematically defined by one or more *objective functions*. An objective function describes the performance parameter in terms of the design variables referring to the stress conditions of the component (F), its geometry (G) and the properties of the material it is made of (M).

$$P = f(F, G, M) \tag{1.5}$$

In most cases, the variables F and G represent respectively the requirements (load conditions) and the constraints (shape and dimensions) of the engineering problem. Therefore, the optimization of the component performance can be primarily obtained acting on the material. The selection of the best performing material involves the identification of the *material index* MI that characterizes the performance parameter P and that is maximized or minimized by the selected material.

In order to get through this procedure more quickly and effectively, particularly in the case of a large number of alternatives, it is possible to superimpose the indices over a bubble diagram (Ashby plot) to conduct a graphic selection. Figure 1.9 shows the bubble diagram for a selection based on material stiffness. Alternative materials are represented by bubbles on the diagram and three material indices are superimposed: each index is graphically reported as a straight line with a slope depending on the loading condition of the component. Each material is represented by an ellipse whose semiaxes are defined by the properties on the diagram axes, here characterized by distributions of values.

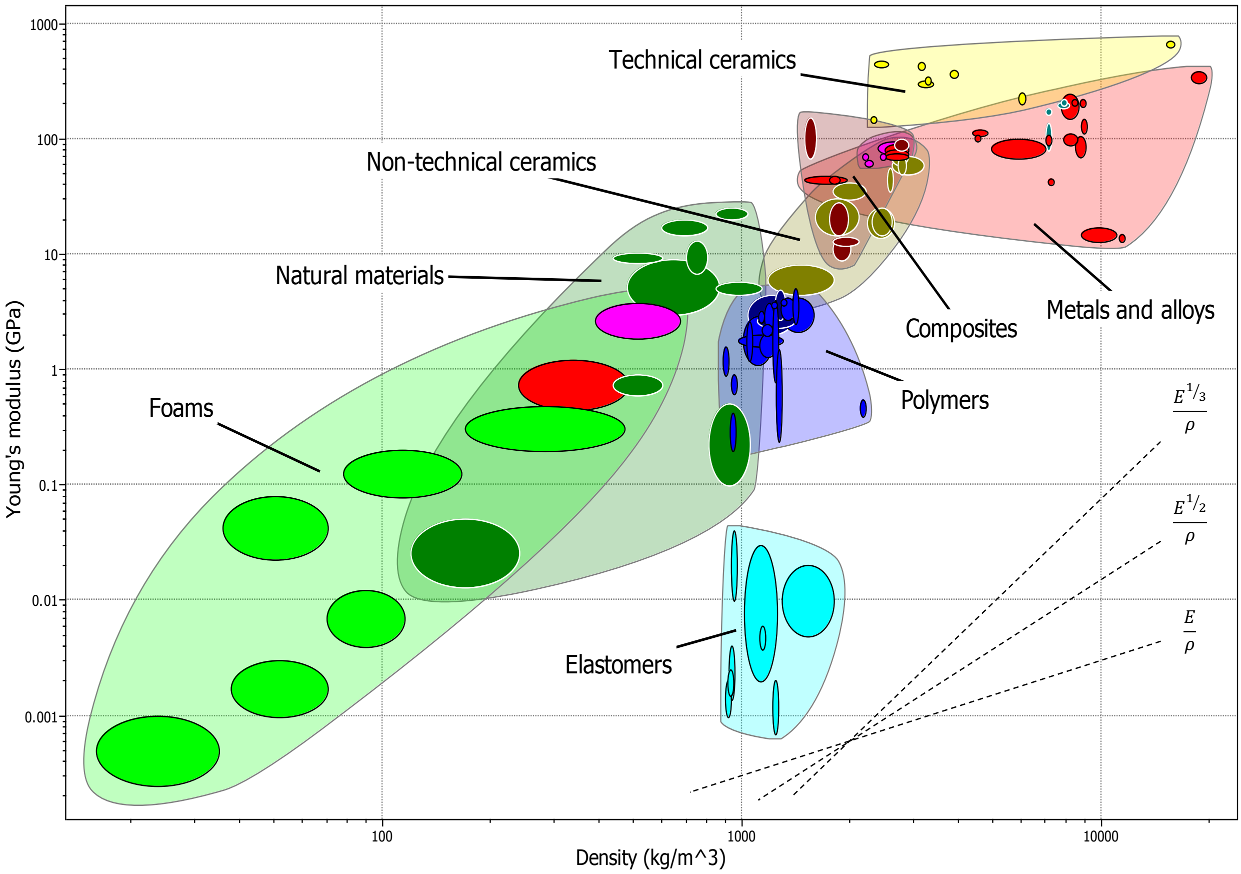

Figure 1.9 - Ashby plot for a materials selection based on stiffness. Three material indices, corresponding to different loading condition of the component, are superimposed as straight lines with a different slope.

In Figure 1.9, each material is characterized by a distribution of values due to microstructure and composition variability, diversified supplies, etc. Therefore, the environmental performances of a material have to include uncertainty as well.

1.8 ECODESIGN

The Ecodesign approach can be defined as a way to design with particular consideration for the environmental and social impacts of a product during its overall life cycle. It can also put in contact the LCT application to the design process and this aspect is widely discussed in the literature.

According to Karlsson and Luttropp (2006), Ecodesign can be summarized as a concept including human sustainability priorities together with business interrelations. Its main objective is to reduce environmental impacts in the improvement of product development methods. This approach also includes a more open ambition to use inspiration from a positive examples of smart products and methods, effective system solutions and attractive designs. However, a definition of sustainable product development is not available. The two authors pointed out that the tools in Ecodesign are not as important as specification and goal setting in early product development phases. Therefore, the way to organize product developments is crucial in order to reach higher degrees of sustainability. In this context, the interrelations between resources (materials and energy) and functionality of products and services must be enhanced.

In a following work, Luttropp and Lagerstedt (2006) discussed about the use of Ecodesign. According to their research, the most important moment in product development is when demands and specifications are decided for the product that is being planned. The specification defines the goal for the product development process and it is a very important opportunity for the continuing work and for environmentally requirements that have to be addressed in the product development phase. Designers have a possible approach for LCT and sustainable product development through Ecodesign. Many tools have been developed in order to help designers to reach environmentally sustainable designs, but most tools are barely used because of a lack of requirements in specifications for products. The authors stated that the lack of market demand for environmentally improved products is a crucial factor: if there is no demand for improved environmental performance, then there is no need for Ecodesign tools.

1.8.1 Design for environment

Another approach similar to Ecodesign is Design for Environment (DfE). Effectively, both Ecodesign and DfE use specific design approaches with the goal to reduce the overall human health and environmental impact of a product, process or service, where impacts are considered with a life cycle perspective. However, Lindajl et al. (2000) recalled the difficulty in applying these methods, stating that in the beginning of the design process knowledge about the product is limited. The information accessible is in general only qualitative, while many methods require quantitative data, something available only in the later phases of the design process. This hampers the successful application of DfE, Ecodesign and, more in general, life cycle studies. Obviously, it is important to get the results as early as possible in the design process before the modification cost becomes prohibitive and the freedom of action becomes too limited.

With Design for Environment it is also possible to identify a US Environmental Protection Agency (EPA)[2] program created in 1992. The target of this program is to prevent pollution and the associated risks for humans and the environment; through Design for Environment it is possible to:

- label industrial and institutional products with safer product labeling;
- define best practices for several products or services or systems;
- identify safer chemicals and life cycle considerations.

1.8.2 Environmental effect analysis (EEA)

Another alternative to Ecodesign is represented by the Environmental Effect Analysis (EEA). The EEA method was primarily developed by the Swedish consulting agency HRM/Ritline AB[3] and has been further implemented in collaboration with other Swedish enterprises and Universities since 1996. EEA is a modification of the quality assurance method Failure Mode and Effect Analysis (FMEA, a potential failure risks evaluation model) and it emphasizes environmental effects during normal operations.

EEA is generally used to identify and assess potential environmental impact risks along the different phases of the life cycle of a product, aiming to take corrective and preventive actions to minimize the environmental burden.

1.8.3 Ecodesign directive

Ecodesign was also used by the European Commission to develop a series of rules and recommendations for sustainable development. For instance, the Ecodesign Directive provides with consistent EU-wide rules for improving the environmental performance of energy related products (ERPs) through Ecodesign. According to the European Commission[4], one of the main targets of this directive is to prevent various and disparate national legislations on the environmental performance of these products from becoming obstacles to the intra-EU trade. This should benefit both businesses and consumers, by enhancing product quality and environmental protection and by facilitating free movement of goods across the EU.

Energy related products (the use of which has an impact on energy consumption) account for a large proportion of the energy consumption in the EU and include:

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2 http://www.epa.gov/dfe/
3 http://www.hrmengineering.se/en/welcome
4 http://ec.europa.eu/enterprise/policies/sustainable-business/ecodesign/

- Energy-using products (EUPs), which use, generate, transfer or measure energy (electricity, gas, fossil fuel), such as boilers, computers, televisions, transformers, industrial fans, industrial furnaces etc.
- Other energy related products (ERPs) which do not use energy but have an impact on energy and can therefore contribute to saving energy, such as windows, insulation material, shower heads, taps etc. The Directive is under the responsibility of *Directorate-general* Enterprise and Industry and *Directorate-general* Energy.

2 PROBABILISTIC UNDERSPECIFICATION

In the residential building sector, the application of LCA is often considered cumbersome because of the complexity of the data collection (generally only available once the design itself is already fully developed and the final construction documents are ready) and the selection of "proxy data" from LCA databases during the modeling phase (the life cycle inventory analysis consists of a collection of input/output data with regard to the system being studied). Therefore, LCA is typically applied by practitioners and designers at the end of a design process, excluding *de facto* the possibility of obtaining environmental results and using them to drive decisions during the early concept or schematic design phase. For the construction sector in particular, this represents a limitation because the use of LCA once a design is almost fully developed is relatively useless, especially if LCA was intended to support decision-making. One possible way to streamline LCA use is to work with the *probabilistic underspecification* approach to create "low-fidelity" categories for use during LCI analysis at the early concept design phases and to address the level of uncertainty in the results at the same time.

2.1 RESEARCH QUESTION

The research question arises from the need to support the overall design process (and not only the final design) with a streamlined implementation of LCA. Ideally, LCA can be used to explore and innovate at the early design stage, when few parameters are available (i.e., the basic geometry, the location, number of stories, etc.) but a broad selection of options for a design is still possible. To answer this research question, the probabilistic underspecification approach was implemented for a series of case studies to test possible applications at different phases of the design process (from the early design stage to the final construction documents), with particular attention to the analysis of uncertainty in the final results. Here, the intended final target consists of the development of an algorithm that provides a wide range of life cycle impacts (expressed as probabilistic distributions) starting from an initial set of specific parameters of a building design. Moreover, the proposed method aims to achieve effectiveness in the results, that is to say that results are obtained within a defined interval of confidence. In the same process, efficiency is achieved, as the need for data collection is lowered.

2.2 METHODOLOGY

To implement a streamlined LCA approach able to support a design process, the work on the probabilistic underspecification presented by Olivetti et al. (2013) was considered as starting point. Olivetti e al. introduced Probabilistic Underspecification as an option to simplify the characterization (specification) of the system under analysis (data collection and LCA modeling), using structured, nested groups of LCA dataset. With this approach, a system can be characterized by available information about the characteristics of materials rather than by specific process-based data, then it is fitted into a hierarchical data structure, Monte Carlo simulation is used to sample all the possible proxy values that correspond with the group identified in the hierarchical data structure (Reis 2013; Olivetti et al. 2013). This approach was used as a viable method both for streamlining and decision-making under uncertainty. Several building assemblies have been analyzed and probabilistic underspecification was used to obtain distributions of environmental impacts for each building assembly, at different levels of specificity. Elaborations and the adopted method are explained hereinafter.

2.2.1 Scope definition

The scope of this work consists of a *cradle-to-gate* LCA applied to residential building assemblies. A *building assembly* is here defined as a structural element of a building and can be both an exterior and an interior object. Examples of building assemblies are exterior and interior walls, foundations, openings (windows and doors), floors, roofs and finishes.

The overall algorithm based on this method will consider all the phases of a building life cycle, in particular the "operational energy" (this is to say the operational energy consumption for heating, cooling, lighting and cooking) and other phases of the "embodied phase" (such as initial construction, maintenance, repairs, replacements, demolition, end of life, transportation), with a final purpose to provide trade-offs between these two main phases of the building life cycle, using a holistic approach. However, this work is particularly focused on the first part of the "embodied phase", a cradle-to-gate analysis of building assemblies, for two reasons. First of all because codes are becoming more stringent and the demand for energy efficient buildings is increasing. As a result, it is becoming more relevant to consider the embodied phase as part of building codes and standards, raising the need to analyze possibilities for improvement and to provide guidelines for material selection, both during the Ecodesign of new buildings and the rehabilitation of existing buildings (Zabalza Bribián et al. 2011). Secondly, but not less important, because studies have revealed growing significance of embodied energy inherent in buildings and have demonstrated its relationship to carbon emissions (Dixit et al. 2012). Previous works have emphasized the significance of embodied energy and have acknowledged its relative proportion of total energy, which is growing with the emergence of more energy efficient buildings (Frey 2008; Plank 2008). Elaborations related to other stages of the building life cycle will be presented within future works of the Concrete Sustainability Hub[5].

2.2.2 Data collection

In order to implement this approach for the residential construction sector, the attention was focused on materials and building assemblies typically adopted in the US residential sector. The first step of the

[5] https://cshub.mit.edu/

procedure consists of a data collection of different LCA datasets of construction materials from relevant databases. These datasets provide LCI and LCIA of materials using a cradle-to-gate approach (datasets within these databases also known as *ecoprofiles*). Databases used for this part were EcoInvent[6], PE International Professional Database[7], USLCI[8] and Athena Sustainable Materials Institute[9]. A database of materials was initially populated with 580 datasets (then reduced to 530, excluding repetitions, errors and outliers) and finally completed using LCIA information, based on the TRACI assessment method with a reference unit of 1 kg of mass for each dataset (conversions were made using information available directly from the specific database or from RS Means Building Cost Data (RSMeans Engineering Department 2013)), and categories defined by the Construction Specifications Institute and Construction Specification Canada[10].

2.2.3 Initial assessment

TRACI version 2.1 was used to assess the environmental impacts of materials and assemblies. Due to a lack of information in some LCA tools and databases (Athena Impact Estimator for Buildings 4.5, for example) specific impact categories were not considered to test this approach (such as ozone depletion, ecotoxicity, human health cancer effects, human health non-cancer effects and fossil fuel depletion). Normalization, grouping and weighting were not contemplated. The reference unit used for the assessment of materials is the unit of mass (1 kg), while the dimension used for building assemblies is the assembly area (1 m^2).

2.2.4 Taxonomy

In biology, taxonomy consists of defining groups of biological organisms on the basis of shared characteristics. Here, taxonomy is used to classify materials and assemblies on the basis of properties and final uses. The classification required by probabilistic underspecification has been structured using (and, where necessary, adapting) the MasterFormat® structure defined by the Construction Specifications Institute (CSI) (Construction Specifications Institute 2014).

[6] http://www.ecoinvent.ch/
[7] http://www.gabi-software.com
[8] http://www.nrel.gov/lci/
[9] http://www.athenasmi.org/
[10] http://www.csinet.org/

```
M1
00 00 00 Procurement and Contracting Requirements
01 00 00 General Requirements
02 00 00 Existing Conditions
03 00 00 Concrete
04 00 00 Masonry
05 00 00 Metals
07 00 00 Thermal and Moisture Protection
|          M2
|———▶ 07 10 00 Dampproofing and Waterproofing
|———▶ 07 20 00 Thermal Protection
:          |          M3
:          |———▶ 07 21 00 Thermal Insulation
:          :          |          M4
:          :          |———▶ 07 21 13 Board Insulation
:          :          :          |          M5
:          :          :          |———▶ Cork slab, at plant/RER U
:          :          :          |———▶ Foam glass, at plant/RER U
:          :          :          |———▶ Polystyrene foam slab, 100% recycled, at plant/CH U
:          :          :          |———▶ Polystyrene foam slab, at plant/RER U
:          :          :          |———▶ Polystyrene, extruded (XPS), at plant/RER U
:          :          :          |———▶ Urea formaldehyde foam slab, hard, at plant/CH U
:          :          :          |———▶ Polyisocyanurate (PIR high-density foam) PE
:          :          :          |———▶ Expanded Polystyrene
:          :          :          |———▶ Extruded Polystyrene
:          :          :          |———▶ Polyiso Foam Board (unfaced)
:          :          :                …
:          :          |———▶ 07 21 16 Blanket Insulation
:          :          |———▶ 07 21 19 Foamed-In-Place Insulation
:          :          |———▶ 07 21 23 Loose-Fill Insulation
:          :          |———▶ 07 21 26 Blown Insulation
:          :          |———▶ 07 21 29 Sprayed Insulation
:          :          |———▶ 07 21 53 Reflective Insulation
:          |———▶ 07 22 00 Roof and Deck Insulation
:          |———▶ 07 24 00 Exterior Insulation and Finish Systems
|———▶ 07 25 00 Weather Barriers
|———▶ 07 30 00 Steep Slope Roofing
|———▶ 07 40 00 Roofing and Siding Panels
|———▶ 07 50 00 Membrane Roofing
|———▶ 07 60 00 Flashing and Sheet Metal
|———▶ 07 70 00 Roof and Wall Specialties and Accessories
|———▶ 07 80 00 Fire and Smoke Protection
|———▶ 07 90 00 Joint Protection
06 00 00 Wood, Plastics, and Composites
08 00 00 Openings
09 00 00 Finishes
…
```

Figure 2.1 - MasterFormat® structure adapted to classify LCA datasets (M5) in nested groups. Polystyrene, extruded (XPS), at plant/RER is the single entry that can be then categorized at different levels of specificity.

MasterFormat® is a standard for organizing specifications and other written information for building projects in the U.S. and Canada. It is organized in different main divisions (e.g., 03 00 00 concrete, 04 00 00 masonry, 05 00 00 metals, 06 00 00 wood, plastics and composites, 07 00 00 thermal and moisture protection, 08 00 00 openings and 09 00 00 finishes) and nested sub-divisions, providing therefore a structured hierarchy for materials and assemblies or, more in general, for all the activities of a construction site. An additional division was added to this structure, in order to group basic materials (clinker, minerals, chemicals, etc.) not directly used in a construction site, but inherent the building sector.

Therefore, each dataset of the materials database was classified using a main division (very generic classification) and other sub-divisions (more specific classification), so as to obtain a hierarchical categorization scheme. For example the dataset "Polystyrene, extruded (XPS), at plant/RER U", available in EcoInvent, is classified as "Thermal and moisture protection" (low level of specificity, category with a total of 134 datasets), "Thermal insulation" (medium level of specificity, 52 datasets) and "Insulation board" (high level of specificity, 19 datasets). Eventually, the individual material datasets and their environmental impacts (referred to the unit of mass) were categorized into five hierarchical levels of specificity, from M1 to M5 with M1 being the first and most general classification (the broad class, like the category "Thermal and moisture protection") and M5 being the most specified (individual entries by LCA databases, such as the dataset "Polystyrene, extruded (XPS), at plant/RER U"). Figure 2.1 gives an idea of the hierarchical categorization scheme.

2.2.5 Monte Carlo simulations

The material database was used to model building assemblies for which bills of materials (BOM) were collected: exterior and interior walls, foundations, doors, windows, roofs and floors. For each assembly, each material of the BOM has been modeled using a specific LCA dataset (corresponding to M5 level) and then a Monte Carlo simulation with 1000 runs was used to obtain a distribution of results for the impact categories, using a reference unit of 1 m^2 of building assembly. Even though M5 entries contain information about specific material impacts, uncertainty is present for a series of reason, since possible perturbation sources are due to measurement instruments, reliability, completeness, application, temporal and geographic correlation of data (Frischknecht et al. 2004; Olivetti et al. 2013).

In LCI definition, a log normal distribution was used to define physical quantities (components of the BOM) and the standard deviation defined a perturbation term, according to the pedigree matrix described by Weidema et al. (Weidema and Wesnaes 1996; Weidema 1998; Weidema 2000). Once obtained this reference results characterized by the highest level of specification, from the LCA point of view, the Probabilistic Underspecification approach was adopted in order to obtain, for the same building assembly, distribution of results at more generic levels of specificity (low-fidelity characterization of the BOM).

2.2.6 Probabilistic underspecification based on uncertainty analysis

The probabilistic underspecification approach aims to be an effective (reasonably accurate) and efficient (reduced need to collect data) streamlining approach (Olivetti et al. 2013). It is defined as a way to implement the use of surrogate data (data from literature or, more in general, other sources not including primary data collection) within LCI analysis and to limit data collection for defining a BOM. The low-fidelity characterization of a BOM and the uncertainty associated with these low levels of fidelity are systematically quantified through underspecification, using the hierarchical classification of each material (Olivetti et al. 2013).

Olivetti et al. proposed this approach as a way to use more generalized materials (or processes) to specify a surrogate LCI, instead of proxy data and also assumed that using an underspecified level rather than proximal process may reduce bias introduced by individual's overconfidence in their knowledge and abilities to classify or categorize activities or materials. Furthermore, experts differ in their knowledge and there has been little study on which are the most appropriate criteria for choosing proxies (Subramanian et al. 2012; Reis 2013). The BOM of a building assembly, which consists of assembly components' mass and materials, can be defined at each level of specificity (from M1 to M5).

The LCA simulation model used specific LCA datasets at M5 and then underspecified from M4 to M1, by means of a random selection of a M5 dataset available in the low-fidelity category list, at M1, M2, M3 and M4. A specific dataset out of the list is chosen for each run of the simulation; in this way, decreasing level is accompanied by less specificity.

A computational tool, Oracle Crystal Ball[11], was used to run Monte Carlo simulations and to obtain distributions of environmental burden, thanks to the generation of impact values for the each component (material) of a BOM (and for each impact category). Then, impact values for the assembly are obtained by aggregation, using Equation (1.1). Table 2.1 provides an example of Probabilistic Underspecification levels (from M5 to M3) for a given building assembly (Insulated Concrete Form wall, ICF).

The probabilistic underspecification is therefore able to estimate the uncertainty associated with the environmental impacts of each assembly, at each level of specificity. As specificity decreases (i.e., moving from M5 to M1), data variability rises and uncertainty increases. On the other hand, using low-fidelity category allows to have environmental results distributions when a design is not developed enough to draw a BOM. Thanks to this approach, comparisons between alternative options or designs become possible and choices can be made with a certain confidential level.

[11] http://www.oracle.com/technetwork/middleware/crystalball/overview/index.html

Table 2.1 - Bill of materials, LCA datasets (M5) and probabilistic underspecification categories (M3 and M4) for ICF wall, with 0,5" (1,27 cm) of exterior stucco, 2" (5,08 cm) of insulation, 4" (10,16 cm) of concrete, other 2" (5,08 cm) of insulation and 0,5" (1,27 cm) of gypsum board.

BOM	M3	M4	M5	Mass [kg]
	Underspecified categories		*LCA dataset level*	
Layer 01	Exterior	Stucco	Stucco, at plant/CH U	18.29
Layer 02	Thermal insulation	Board insulation/EPS	Polystyrene foam slab, at plant/RER U	1.52
Layer 03	Cast in place	Concrete 2400 kg/m^3	Concrete, normal, at plant/CH U	241.81
Layer 04	Thermal insulation	Board insulation/EPS	Polystyrene foam slab, at plant/RER U	1.52
Layer 05	Interior board	Gypsum board	Gypsum fibre board, at plant/CH U	14.29
Layer 06	Connectors	Plastic connectors	Polypropylene, granulate, at plant/RER U	0.52
Layer 07	Reinforcing steel	Rebar steel	Reinforcing steel, at plant/RER U	1.11
Layer 08	Support	Joint-compound	Joint compound	1.10
Layer 09	Support	Paper	Paper tape	0.01
Layer 10	Rough carpentry	Soft-Dried Wood	Sawn timber, softwood, raw, kiln dried, u=20%, at plant/RER U	7.24
Layer 11	Interior	Paint	Alkyd paint, white, 60% in H2O, at plant/RER U	0.08

2.3 CASE STUDIES

Based on the guidelines defined by the American Institute of Architects (Bayer et al. 2010), a survey conducted by the Concrete Sustainability Hub (CSHub 2013) and the experience of the research team, the building design process has been divided into 5 different phases: (1) *Conceptual design*, in which designers draw the basic geometry of a building and basic parameters (locations, number of stories, etc.) are known; (2) *Schematic design*, in which parameters in the first phase are consolidated and first details are defined (type of walls, number and position of openings, foundations, type of roofs, etc.); (3) *Design development* in which designers study the performance of building assemblies (for example the thickness of different layers of materials and the consequent thermal resistance); (4) *Construction documents*, in which details about a building and its assemblies are defined (specific kind of insulation, specific kind of glass, exterior finishes, etc.) according to the CSI divisions; (5) *Final construction documents*, in which designers are able to draw a complete and detailed BOM and each item can be represented by a proxy LCA dataset in an LCA model.

```
L1
Exterior walls (52)
|          L2
|———► Concrete Masonry Units (18)
|———► Insulated Concrete Forms (12)
:          |          L3
:          |———► 2" insulation, 4" concrete, 2" insulation
:          |———► 3" insulation, 4" concrete, 3" insulation
:          |———► 4" insulation, 4" concrete, 4" insulation
:          |———► 2" insulation, 6" concrete, 2" insulation
:          |———► 3" insulation, 6" concrete, 3" insulation
:          |———► 4" insulation, 6" concrete, 4" insulation
:          |———► …
|———► Precast Concrete walls (5)
|———► Structural insulated panels (5)
|———► Wood stud walls (12)
Interior walls (4)
|          L2
|———► Insulated walls (2)
|———► Non-insulated walls (2)
Foundations (49)
|          L2
|———► Concrete Masonry Units (24)
|———► Cast in place (8)
|———► Insulated Concrete Forms (9)
|———► Slab on grade (8)
Doors (7)
|          L2
|———► Glazed doors (3)
|———► Unglazed doors (4)
Windows (48)
|          L2
|———► Aluminum frame (8)
|———► Fiberglass frame (8)
|———► PVC frame (8)
|———► Wood frame (8)
|———► Wood+Aluminum frame (8)
|———► Wood+vinyl frame (8)
Roofs and ceilings (96)
|          L2
|———► Wood joists ceilings (12)
|———► Wood joists roofs (36)
|———► I-joists ceilings (12)
|———► I-joists roofs (36)
Floors (12)
|          L2
|———► Wood joists floors (4)
|———► Wood truss (8)
Exterior finishes (29)
|          L2
|———► Wall finishes (18)
|———► Roof finishes (11)
```

Figure 2.2 - Hierarchical structure for building assemblies. Single assemblies are analyzed using materials at M3, M4 and M5 (LCA datasets). Then assemblies are grouped to form L2 categories and L1 macro-categories. Numbers in brackets refer to the volume of the population.

The case studies analyzed represent a series of building assemblies (exterior walls, interior walls, foundations, roofs, floors, windows, doors, exterior finishes) that can be used to obtain distributions of environmental results, using a cradle-to-gate approach, along the five phases of building design process. From phase 1 to phase 5 designers increment the level of specificity and decrease the variation of options, therefore uncertainty in results decreases. To test the functionality of this approach, almost three hundred different building assemblies typically used in the U.S. residential sector were analyzed. BOMs and details about residential building assemblies have been collected from the textbook Architectural Graphic Standards for Residential Construction (Hall and Giglio 2010) and from the tools Athena Impact Estimator for Buildings V4.5 and Building Energy Optimization (BEopt) V2.1[12]. For each assembly, a distribution of results is obtained using the highest level of specificity (M5 single entries used for assembly components), here referred as L5. Indeed, during the development of the simulations it was decided to refer to M1-5 classification for materials, while L1-5 are referred here as classification levels for assemblies.

Subsequently, the first step of underspecification was used (M4 materials category) to obtain the assembly level of specificity L4 and finally the second step of underspecification (M3 materials category) to obtain L3. Materials categories M2 and M1 were not used because too generic and because uncertainty would be too difficult to handle. Therefore, L2 and L1 for building assemblies were obtained using the aggregation of result distributions achieved by different building assemblies at L3, as shown in Figure 2.2.

For instance, the analyzed exterior walls were 52 individuals, in total. They are divided into five main typologies (L1 level), commonly used in the residential building sector (Concrete Masonry Units, Insulated Concrete Forms, Precast Concrete walls, Structural Insulated Panels, Wood Stud walls). Usually, information available by a designer during the Concept design (phase 1 of the design process) is probably just an estimation of the assembly area, therefore the corresponding distribution of environmental results for this level is L1 in which the variation of all the 52 walls is included. In phase 2, the available information is supposed to be incremented, at least by a wall typology definition, so L2 will be used. Assuming to use one of these wall typologies, for instance the Insulated concrete forms (ICF), the variation is reduced to 12 walls out of 52, as available in Figure 2.2. During the Design development (phase 3) a specific wall is chosen (1 out of 12 representative of the ICF typology) and therefore L3 is used for that specific wall. In this phase further details are decided, for example specific thickness of different layers of the ICF wall. Thus, a distribution of results is obtained thanks to the use of materials categories at M3. More details are added during phase 4 (for example specific material typologies for different layers) and phase 5 (more detailed information about specific materials). Therefore, L4 and L5 are respectively obtained for the same building assembly (the same ICF chosen in the third step) using material categories at M4 and M5, reducing uncertainty in results to the minimum value for the latter case (single LCA databases).

[12] https://beopt.nrel.gov/

A summary of this example is detailed hereinafter:

(1) Conceptual design. Generic wall at L1. General assembly class, comprehensive of the variation of all the analyzed walls (using categories of materials at M3).
(2) Schematic design. Wall typology specification at L2. Assembly typology, comprehensive of the variation of a sub-group of analyzed walls (using categories of materials at M3).
(3) Design development. Generic single wall specification at L3. A single assembly is analyzed. Distribution of results obtained using categories of materials at M3.
(4) Construction documents. Detailed single wall at L4. A single assembly is analyzed. Distribution of results obtained using categories of materials at M4.
(5) Final construction documents. Fully detailed single wall at L5. A single assembly is analyzed. Distribution of results obtained using LCA datasets of materials at M5.

Figure 2.2 summarizes the building assemblies considered for this work; due to limit of space, L4 and L5 are excluded and L3 is partially provided for ICF walls. Table 2.1 provides the necessary information for a specific ICF wall, analyzed using materials categories from M3 to M5 and therefore providing three distributions of results for the building assembly (from L3 to L5).

2.4 EVALUATION METRICS

2.4.1 Dispersion of results

The median absolute deviation coefficient of variation (MAD-COV) is a measure of data dispersion similar to standard deviation, but more robust to data outliers (Rousseeuw and Croux 2012), has been used as a performance metric. The MAD-COV describes the median percent variation of a dataset from the median value. In equation (2.1), MAD-COV for a generic environmental indicator and a defined level of specificity (Lj, j = 1:5) is obtained using each single environmental result of a Monte Carlo simulation (x_i, i = 1:1000) and the median value of all the 1000 Monte Carlo simulation results (median(X_{Lj})).

$$MAD - COV_{Lj} = \frac{median(\left|x_{iLj} - median\left(X_{Lj}\right)\right|)}{median\left(X_{Lj}\right)} \tag{2.1}$$

Even though the MAD-COV is considered the principal for this study, other performance metrics exist; those considered useful to describe data dispersion and accuracy of results are respectively the coefficient of variation (CV for a generic environmental indicator, equation (2.2)) and the median distance (MD for a generic environmental indicator, equation (2.3)).

$$CV_{Lj} = \frac{standard\ deviation(X_{Lj})}{mean(X_{Lj})} \tag{2.2}$$

$$MD_{Lj} = \frac{|median(X_{Lj}) - median(X_{L5})|}{median(X_{L5})} \tag{2.3}$$

2.4.2 Comparison Indicator

The use of probabilistic underspecification introduces uncertainty and variation in results, a characteristic that can be measured and controlled. Moreover, results at levels L1-L5 allow decision-making at different points of the design process, since LCA results are usually interpreted in a comparative manner (Noshadravan et al. 2013). A Comparison Indicator (CI) was used to evaluate the difference between two alternative designs; CI is defined as the ratio between environmental impacts of two products (Huijbregts et al. 2003). Therefore, the choice driver is not the overall uncertainty in individual assemblies, but the uncertainty in the difference between two building assemblies (design A and design B, in equation (2.4)).

$$CI_{Lj} = \frac{(X_{Lj-design\ A})}{(X_{Lj-design\ B})} \tag{2.4}$$

The probability that design A has lower environmental burden than design B is computable through equation(2.5), in which β is a probability.

$$\beta_{Lj} = P(CI_{Lj} < 1) \tag{2.5}$$

2.5 RESULTS

The ICF wall described in Table 2.1 has chosen to show an example of result distributions (concerning impact such as acidification, eutrophication, global warming, smog creation) at different levels of specificity, obtained thanks to Monte Carlo simulations. Figure 2.3 provides the probabilistic distributions of global warming (GW), starting from a generic L1 wall and finishing with the specific L5 ICF wall, using boxplots. Boxplots are built in this way: the bottom and top of the box are the first and third quartiles (25^{th} and 75^{th} percentiles), the band inside the box is the median (second quartile) and the whiskers' limits represent the 5^{th} percentile and the 95^{th} percentile. As a reminder, for all the simulations the scope of the analysis is limited, at the moment, at the first stage of the "embodied phase" (cradle-to-gate approach).

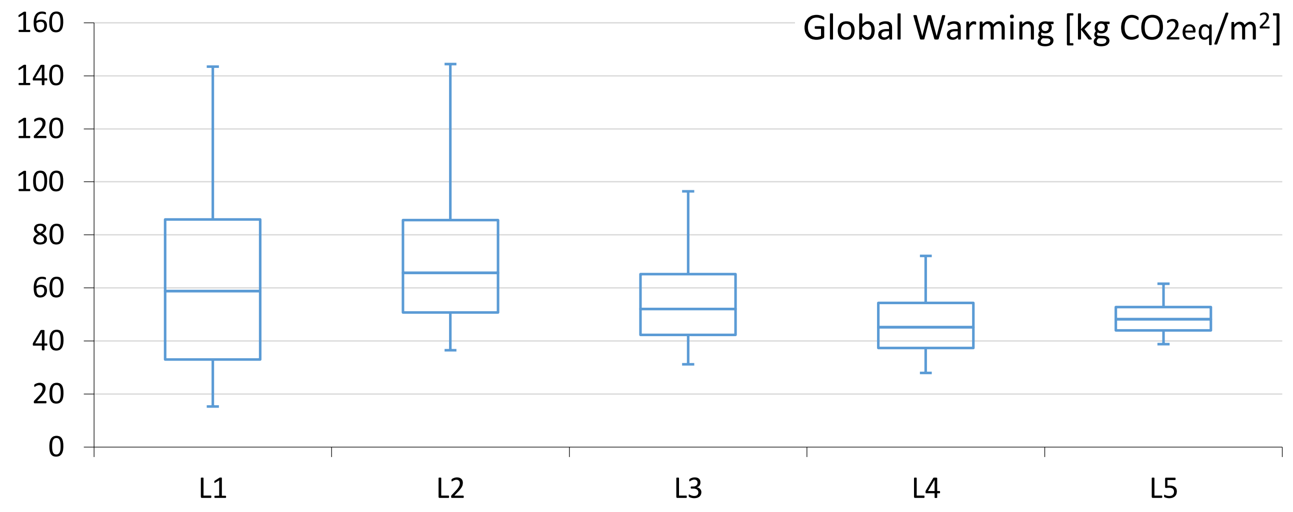


Figure 2.3 - Probabilistic distributions of global warming results applied to an exterior wall (ICF). Typical results from an LCA study are represented by L5, while from L4 to L1 the probabilistic underspecification approach is used.

Boxplots in Figure 2.3 demonstrate a reduced, but still present, uncertainty at L5, with a median GW of 48.2 kg CO_2 eq/m^2 and a standard deviation of 6.7. Using the underspecified categories described in Table 2.1, L4 and L3 results are characterized by a similar median GW (respectively 45.2 and 52.1 kg CO_2 eq/m^2) but a wider distribution, with standard deviations of 13.7 and 20.9. L2 and L1 boxplots appear even larger because of the variation of different assemblies within the same category (12 ICF walls in L2 and 52 exterior walls in L1). Other environmental indicators confirm this trend, as it is possible to appreciate in Figure 2.4, Figure 2.5 and Figure 2.6.

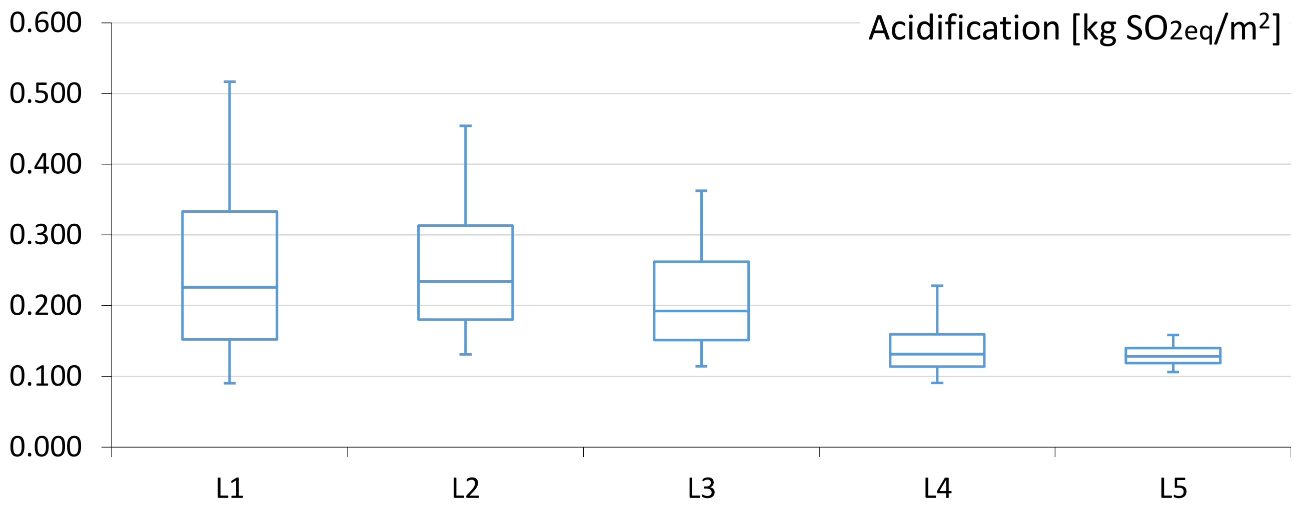


Figure 2.4 - Probabilistic distributions of acidification results applied to an exterior wall (ICF). Typical results from an LCA study are represented by L5, while from L4 to L1 the probabilistic underspecification approach is used.

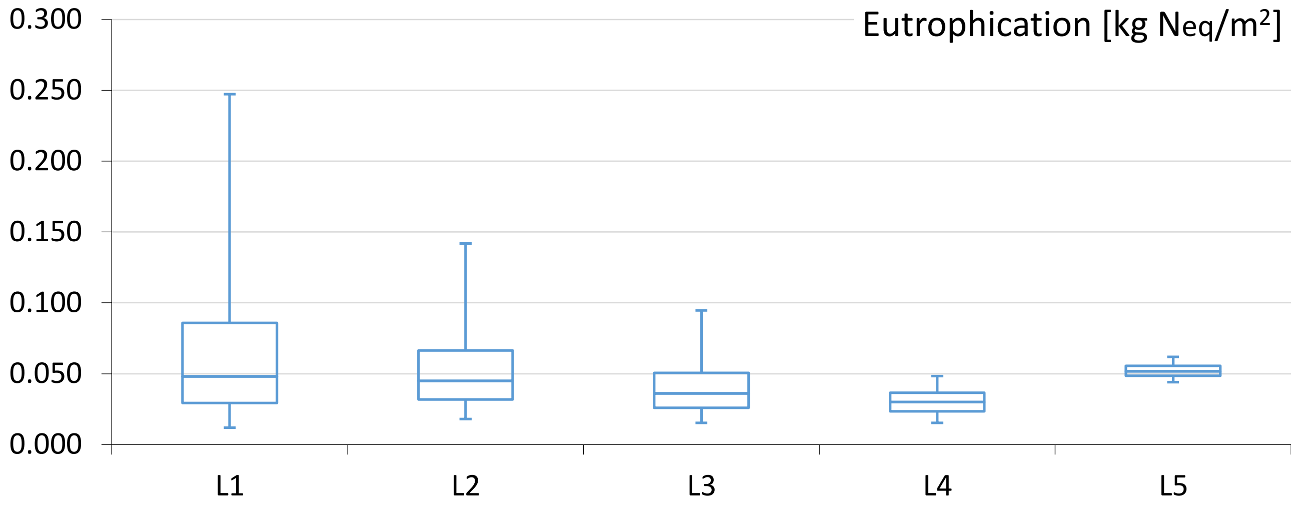


Figure 2.5 - Probabilistic distributions of eutrophication results applied to an exterior wall (ICF). Typical results from an LCA study are represented by L5, while from L4 to L1 the probabilistic underspecification approach is used.

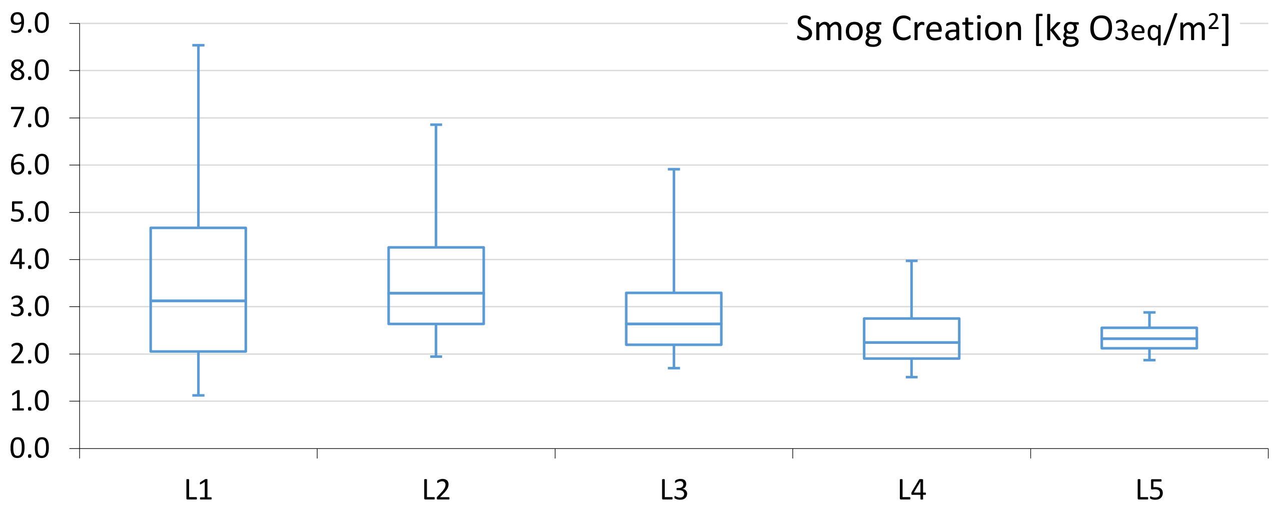
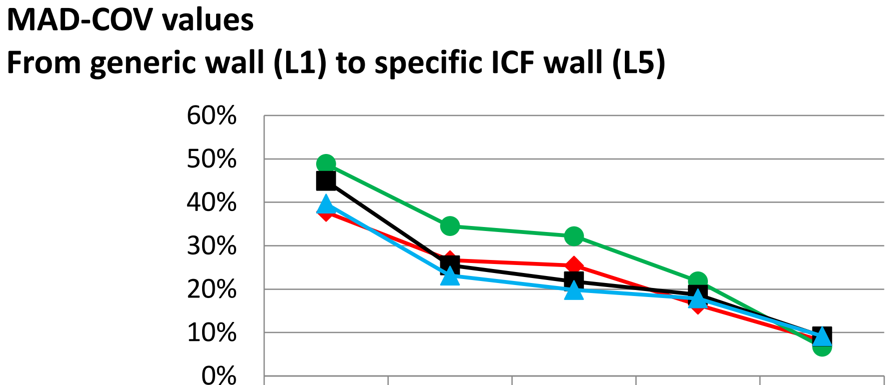


Figure 2.6 - Probabilistic distributions of smog creation results applied to an exterior wall (ICF). Typical results from an LCA study are represented by L5, while from L4 to L1 the probabilistic underspecification approach is used.

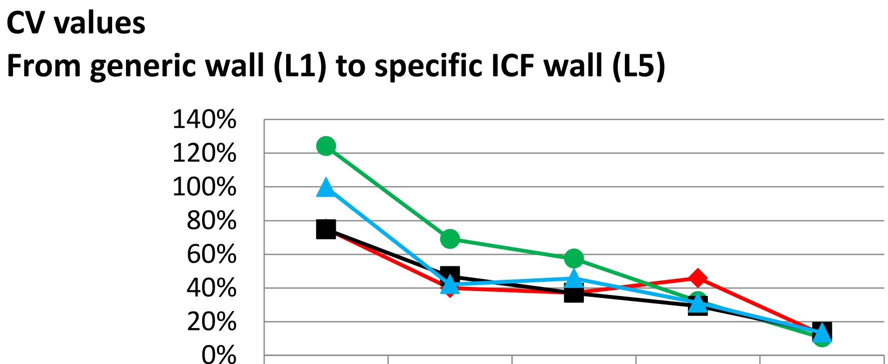
MAD-COV results at different levels and for different environmental indicators are shown in Figure 2.7. Whereas MAD-COV$_{L5}$ is always lower than 10%, recalling again a solid reliability for the highest level of specificity, the trend of results from L4 to L1 is generally growing, even though anomalies can be highlighted, due to the fact that materials are characterized by different environmental impacts and it is possible that environmental indicators for a specific LCA dataset may not be consistent among them.



	L1	L2	L3	L4	L5
Acidification	0.38	0.27	0.25	0.16	0.08
Eutrophication	0.49	0.35	0.32	0.22	0.07
Global Warming	0.45	0.25	0.22	0.19	0.09
Smog creation	0.40	0.23	0.20	0.18	0.09

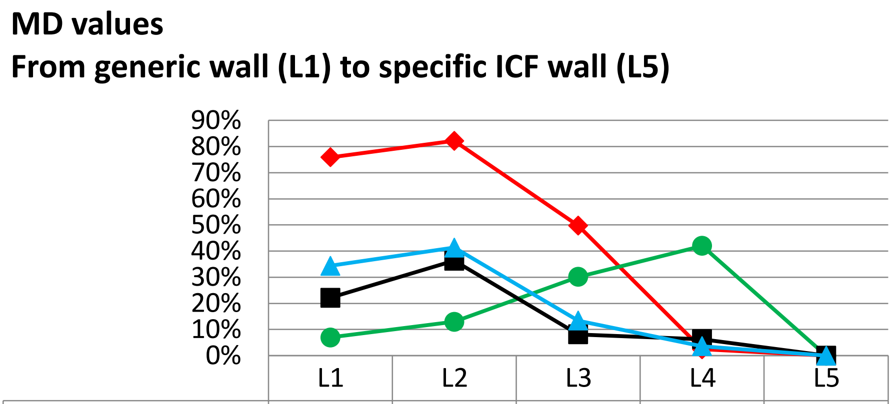
Figure 2.7 - MAD-COV for the environmental impacts at different levels of specificity: From a generic wall (L1) to a specific ICF wall (L5). L2 refers to the ICF wall category.

Figure 2.8 and Figure 2.9 provide results for CV and MD metrics obtained using the ICF case study. Where for CV values the trend is clear and stable for all the environmental categories, MD results present more anomalies due to different materials' environmental performance.



	L1	L2	L3	L4	L5
Acidification	0.75	0.40	0.37	0.46	0.12
Eutrophication	1.24	0.69	0.57	0.32	0.11
Global Warming	0.75	0.47	0.37	0.29	0.14
Smog creation	1.00	0.42	0.46	0.31	0.13

Figure 2.8 - CV for the environmental impacts at different levels of specificity: From a generic wall (L1) to a specific ICF wall (L5). L2 refers to the ICF wall category.



	L1	L2	L3	L4	L5
Acidification	76%	82%	50%	2%	0%
Eutrophication	7%	13%	30%	42%	0%
Global Warming	22%	36%	8%	6%	0%
Smog creation	34%	41%	13%	4%	0%

Figure 2.9 - MD for the environmental impacts at different levels of specificity: From a generic wall (L1) to a specific ICF wall (L5). L2 refers to the ICF wall category.

To show an example of the Comparison Indicator practical utility, the ICF wall described in Table 2.1 (design A) was considered, as well as another ICF wall in which Layer 02 and Layer 04 (Polystyrene foam slab, at plant/RER U) change from a thickness of 2 inches to 4 inches (8 inches in total), clearly defining a higher environmental impact, considering a cradle-to-gate approach. As a matter of fact, at L5 the probability β_{L5} that GW for design A is lower than GW for design B was calculated to be 92%, confirming that, given the same area of 1 m^2 and different amounts of the same material, the best environmental performance is obtainable by the lighter assembly (use phase is not considered). On the other hand, at L3 the probability β_{L3} that GW for design A is lower than GW for design B is just 69%, highlighting an increased uncertainty due to possible variations in the material selection. In this case, the widest source of variation is due to insulation and β_{L3} provides information that this component should be specified in order to have a higher probability, ergo a more robust basis for decision-making. At the same time it is possible, during the design development or other phases of the design process, to test different options and obtain a reliable estimation of final environmental impacts for a building assembly. This approach may be of particular interest for designers since building codes and standards often require to achieve a defined assembly thermal resistance, according to a building typology and a geographical area; with this approach, during the early design stage, it is possible to select a range of building assemblies that satisfy the same performance (thermal resistance, cost, use of recycled materials, use of renewable materials, etc.), compare them by means of the CI and therefore strengthen the decision-making process and simultaneously informing designers about environmental impacts. These two hypothesis are represented in Figure 2.10.

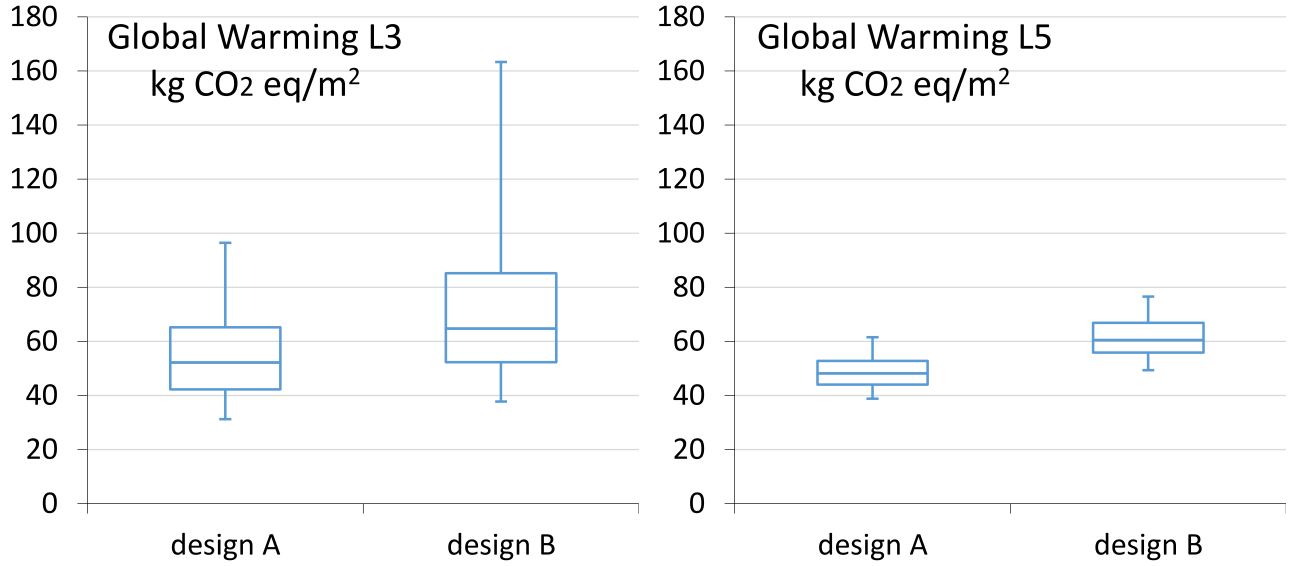
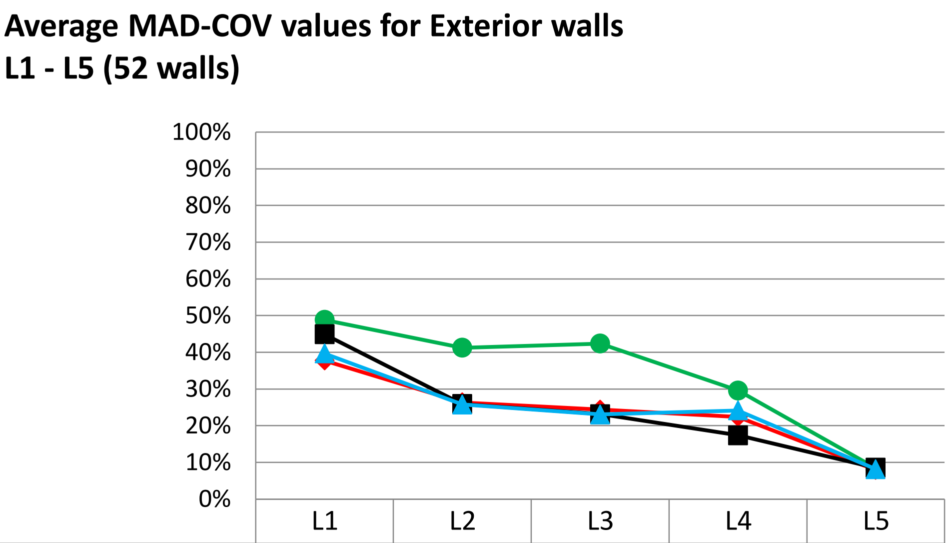


Figure 2.10 - Global warming distributions for design A and design B. On the left hand side distributions represent L3, in which material details are not specified (β = 69%). On the right hand side distributions represent L5, where BOMs are fully specified (β = 92%).

2.5.1 Building assembly typologies

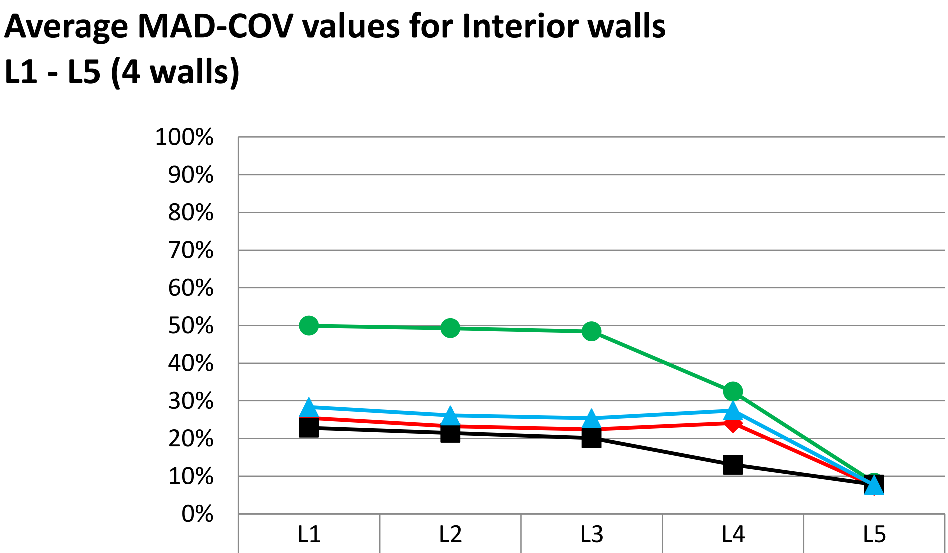
The probabilistic underspecification approach has been used with several residential building assemblies, in order to test its efficiency and effectiveness. For this purpose a MAD-COV metric has been evaluated for each assembly and for each environmental impact category. Average results for 52 exterior walls are reported in Figure 2.11 (from L3 to L5), while at L2 and L1 average MAD-COV values were obtained using category MAD-COV averages (Figure 2.2, 5 wall categories at L2 and one macro-category of exterior walls at L1).

The general trend represented in Figure 2.7 (underspecification relative to a single exterior wall) is generally confirmed by average MAD-COV values of the exterior walls category, even though, as already stated, anomalies can be identified (for Eutrophication average $MAD\text{-}COV_{L2}$ < average $MAD\text{-}COV_{L3}$ and for Smog creation average $MAD\text{-}COV_{L3}$ < average $MAD\text{-}COV_{L4}$). Average MAD-COV values have been calculated also for other building assembly categories and results validate the previous affirmation. From Figure 2.12 to Figure 2.18, average MAD-COV values related to a series of assembly categories are shown for acidification, eutrophication, global warming and smog creation, highlighting the wider data dispersion at L1 and L2.



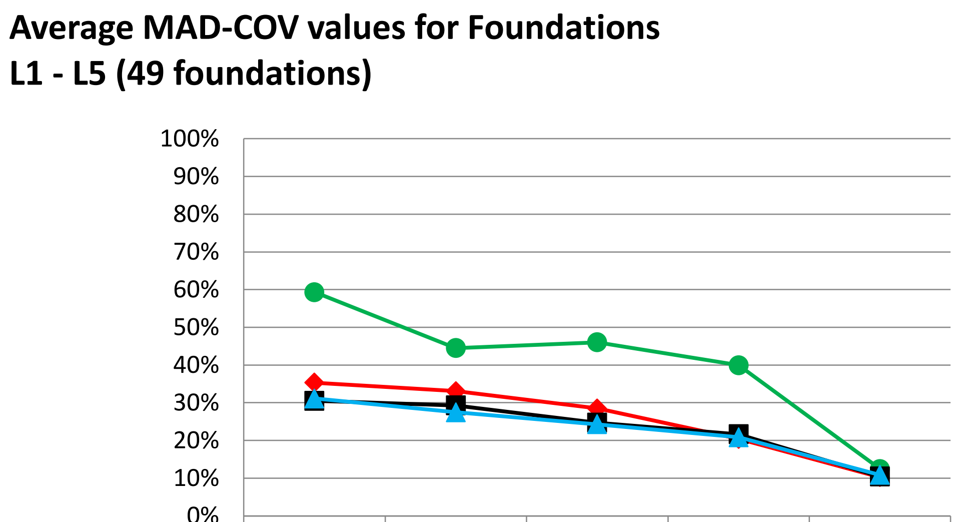
	L1	L2	L3	L4	L5
Acidification	0.38	0.26	0.24	0.22	0.08
Eutrophication	0.49	0.41	0.42	0.30	0.08
Global warming	0.45	0.26	0.23	0.17	0.09
Smog creation	0.40	0.26	0.23	0.24	0.08

Figure 2.11 - Average MAD-COV for exterior walls obtained from the analysis of 52 walls (from L3 to L5), 5 wall typologies (L2) and one macro-category (L1, generic wall).



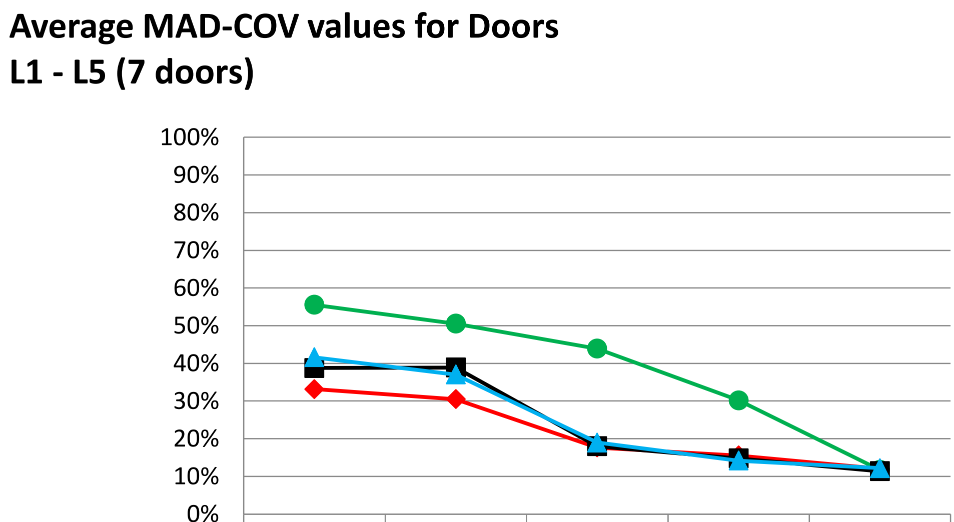
	L1	L2	L3	L4	L5
Acidification	0.25	0.23	0.22	0.24	0.07
Eutrophication	0.50	0.49	0.48	0.32	0.08
Global warming	0.23	0.21	0.20	0.13	0.08
Smog creation	0.28	0.26	0.25	0.27	0.08

Figure 2.12 - Average MAD-COV for interior walls obtained from the analysis of 4 walls (from L3 to L5), 2 wall typologies (L2) and one macro-category (L1, generic wall).



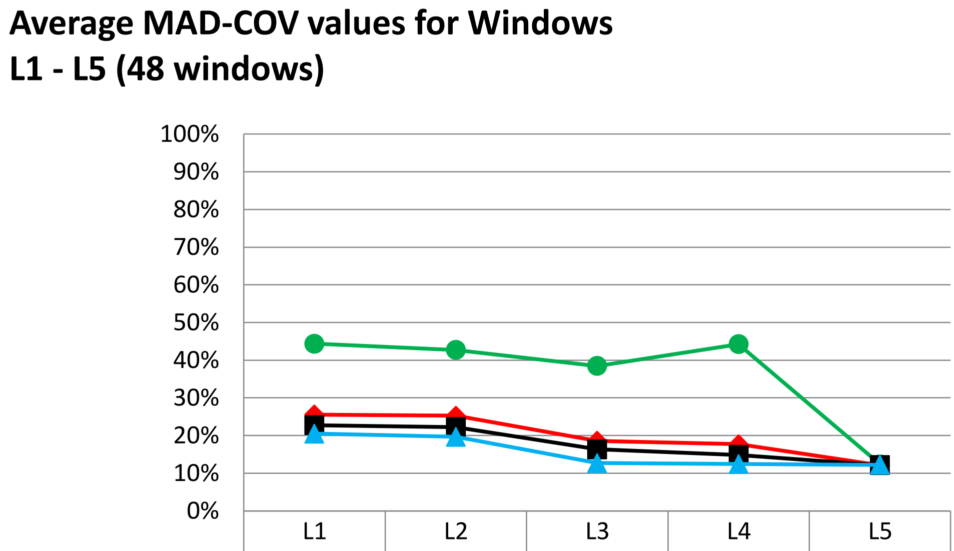
	L1	L2	L3	L4	L5
Acidification	0.35	0.33	0.28	0.20	0.10
Eutrophication	0.59	0.44	0.46	0.40	0.12
Global warming	0.31	0.29	0.25	0.22	0.10
Smog creation	0.31	0.27	0.24	0.21	0.11

Figure 2.13 - Average MAD-COV for foundations obtained from the analysis of 49 foundations (from L3 to L5), 4 typologies (L2) and one macro-category (L1, generic foundations).



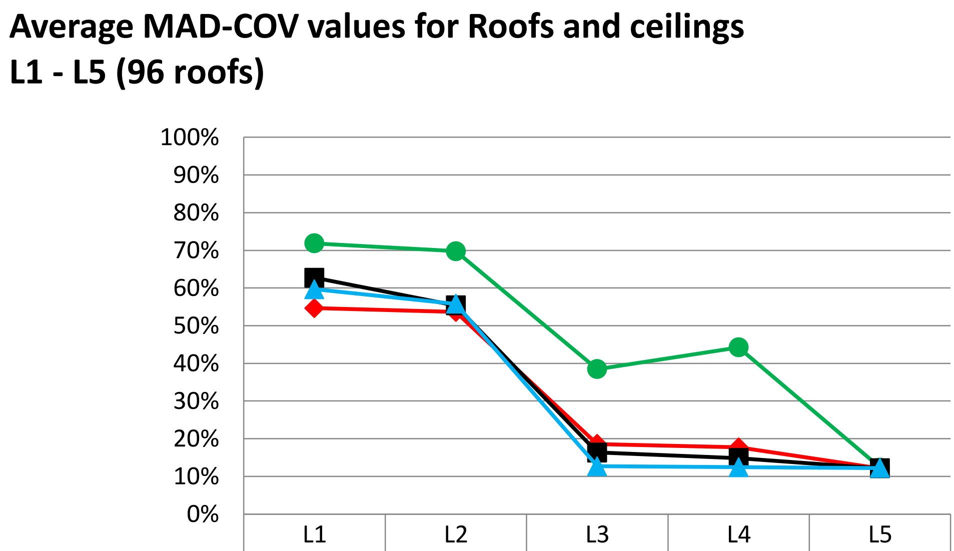
	L1	L2	L3	L4	L5
Acidification	0.33	0.30	0.18	0.16	0.12
Eutrophication	0.56	0.51	0.44	0.30	0.12
Global warming	0.39	0.39	0.18	0.15	0.11
Smog creation	0.42	0.37	0.19	0.14	0.12

Figure 2.14 - Average MAD-COV for doors obtained from the analysis of 7 doors (from L3 to L5), 2 typologies (L2) and one macro-category (L1, generic door).



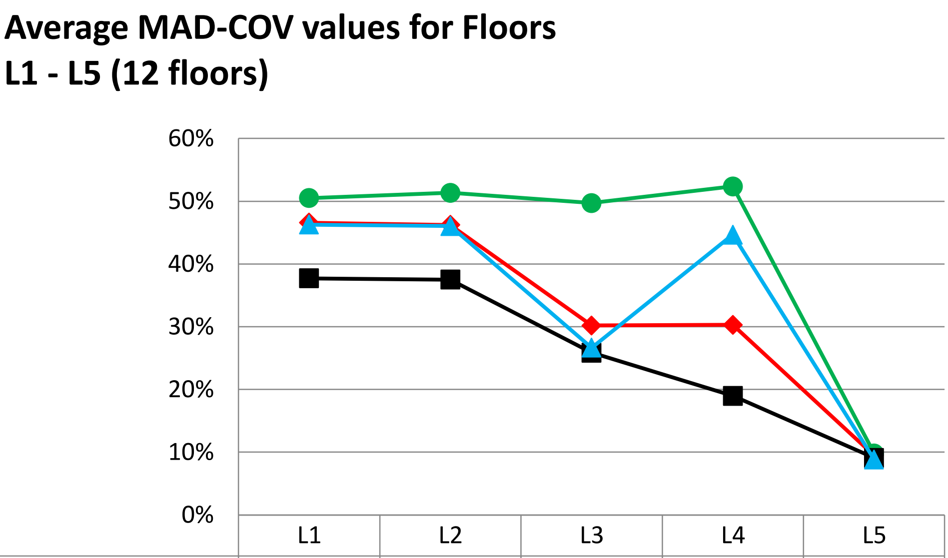
	L1	L2	L3	L4	L5
Acidification	0.26	0.25	0.19	0.18	0.12
Eutrophication	0.44	0.43	0.38	0.44	0.12
Global warming	0.23	0.22	0.16	0.15	0.12
Smog creation	0.20	0.20	0.13	0.12	0.12

Figure 2.15 - Average MAD-COV for windows obtained from the analysis of 48 windows (from L3 to L5), 6 frame typologies (L2) and one macro-category (L1, generic windows).



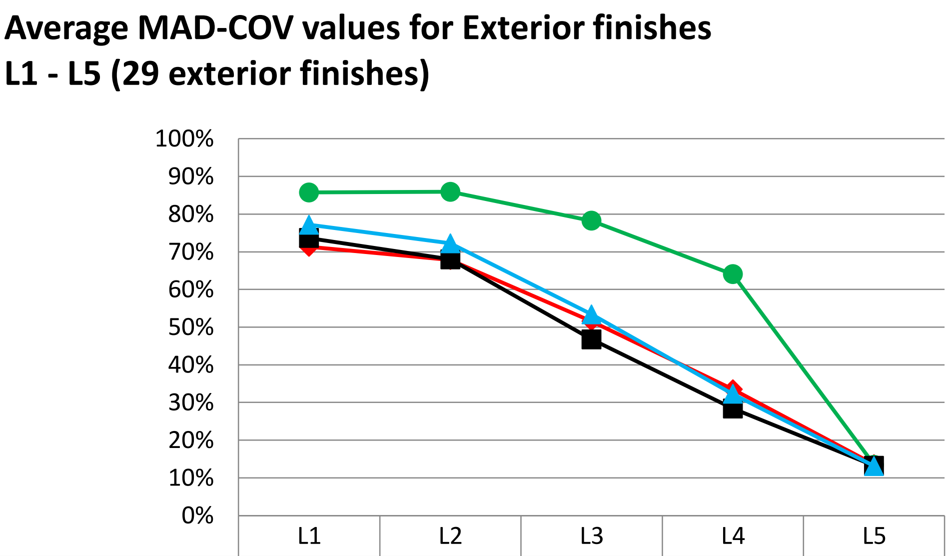
	L1	L2	L3	L4	L5
Acidification	0.55	0.54	0.19	0.18	0.12
Eutrophication	0.72	0.70	0.38	0.44	0.12
Global warming	0.63	0.55	0.16	0.15	0.12
Smog creation	0.60	0.56	0.13	0.12	0.12

Figure 2.16 - Average MAD-COV for roofs and ceilings obtained from the analysis of 96 assemblies (from L3 to L5), 4 typologies (L2) and one macro-category (L1, generic roof).



	L1	L2	L3	L4	L5
Acidification	0.47	0.46	0.30	0.30	0.09
Eutrophication	0.50	0.51	0.50	0.52	0.10
Global warming	0.38	0.38	0.26	0.19	0.09
Smog creation	0.46	0.46	0.27	0.45	0.09

Figure 2.17 - Average MAD-COV for floors obtained from the analysis of 12 assemblies (from L3 to L5), 2 typologies (L2) and one macro-category (L1, generic floor).



	L1	L2	L3	L4	L5
Acidification	0.71	0.68	0.52	0.34	0.14
Eutrophication	0.86	0.86	0.78	0.64	0.13
Global warming	0.74	0.68	0.47	0.28	0.13
Smog creation	0.77	0.72	0.53	0.32	0.13

Figure 2.18 - Average MAD-COV for exterior finishes obtained from the analysis of 29 finishes (from L3 to L5), 2 typologies (L2) and one macro-category (L1, generic exterior finish).

2.5.2 Alternative taxonomy

In order to test the efficiency of the classification structure adopted in this work, M3 and M4 levels for material taxonomy were redefined using price ($/kg) and conductivity (W/m·K) as classifiers. In this way, an alternative taxonomy for construction materials was created and part of the simulations were re-processed. Through data visualization, clusters of materials were formed using the two classifiers, as reported in Table 2.2.

Table 2.2 - Classifiers and clusters of materials used to define an alternative taxonomy.

Price ($/kg)
< 1
1 – 2
2 – 3
3 – 5
> 5

Conductivity (W/m·K)
< 0.05
0.05 – 0.1
0.1 – 0.2
0.2 – 0.4
0.4 – 1.0
1.0 – 3.0
> 3.0

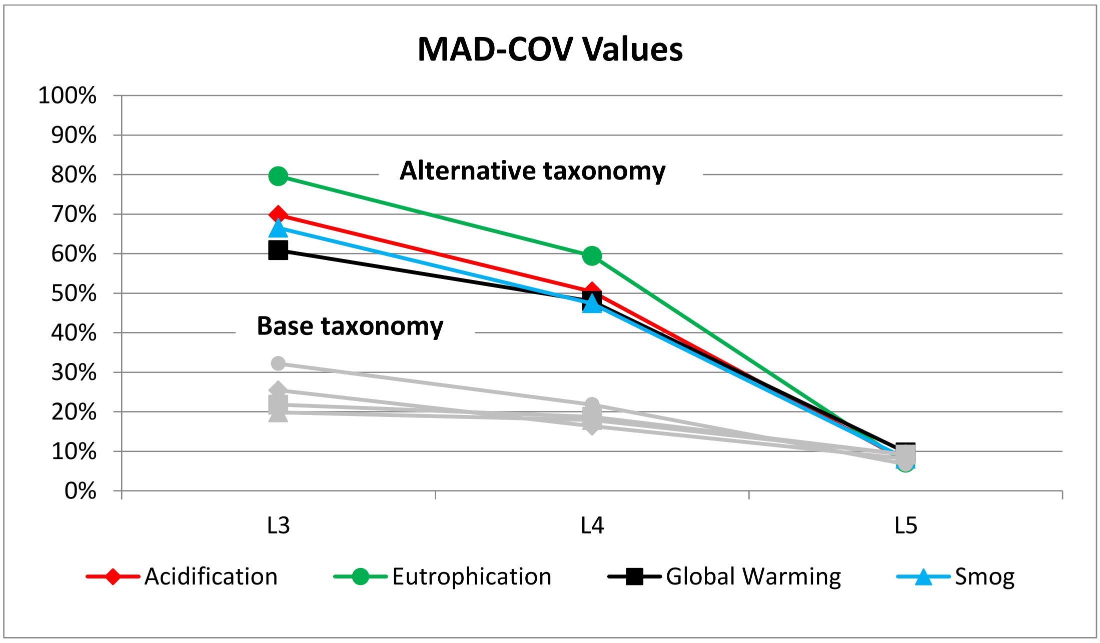


Figure 2.19 - MAD-COV values for an ICF wall (from L3 to L5) analyzed with two possible material taxonomies: Base taxonomy grounded on the CSI specifications and Alternative taxonomy grounded on price (M3) and conductivity (M4) as classifiers.

Simulation results provided different performance metrics and distributions of results. An example of MAD-COV metrics for an ICF wall (the reference wall described in Table 2.1) is represented in Figure 2.19, where the same metrics for the base taxonomy are available for comparison.

2.6 DISCUSSION

The series of tests conducted for this work revealed probabilistic underspecification to be an interesting approach for a streamlined LCA methodology tailored to the building sector. Quantitative results for the relevant environmental categories, processed with uncertainty analysis, can be obtained using low-fidelity categories for materials and building assemblies, demonstrating that LCA can be applied not only when a complete and detailed bill of materials is available but also when fewer details are known. Therefore, decision-making based on this approach at different phases of the design process can be sustained by use of the Comparison Indicator.

In general terms, the approach proved to be efficient because extensive data collection for inventory analysis was not necessary. Further developments that put into practice the use of hybrid models are advisable to test the approach's effectiveness, as designers and architects can probably provide information on building parameters at different levels of detail (see Chapter 3 Probabilistic Triage). It is also desirable that the database of environmental impacts of building assemblies (and categories) be tested by experts (designers and architects) to evaluate the real reduction of cost and time for LCA implementation.

Further work could also investigate the use of a different and possibly more efficient way to structure the taxonomy for materials and for assemblies. Figure 2.12 to Figure 2.18 show how data dispersion at L1 and L2 is wider for some assembly categories but under 30% for others (foundations, interior walls and windows), indicating that a more structured approach can be used to develop materials or assembly taxonomy.

Lee applied the probabilistic underspecification method to a case study and highlighted that poor data structures reduced accuracy in streamlining (Lee 2013), while Reis found that data mining techniques support probabilistic underspecification and streamlined LCA, providing indications on how to develop a material taxonomy able to reduce the error rates on environmental results (Reis 2013).

The data collection phase included a series of classifiers for each material: price, conductivity, density, etc. These classifiers were used to structure an alternative material classification, but this did not bring about an improvement in results. Figure 2.19 shows an example of the higher data dispersion obtained using the Alternative taxonomy. Whereas the average MAD-COV value at L3 is about 25% for the Base taxonomy, it becomes 69% with the Alternative one. At L4 the gap is reduced, but still significant: an average of 19% for the Base taxonomy, 51% for the Alternative taxonomy. Additional research here could be useful, although a structure based on the CSI divisions is probably more efficient for experts in the field.

Ultimately, this work will be part of a larger algorithm under development at the Concrete Sustainability Hub, in which the other parts of the building's life cycle will be included to identify trade-offs among the estimated impacts of the operational use phase, the embodied phase and the end of life. The operational use phase in particular is recognized as a key contributor to the total impact of residential buildings and will be assessed in conjunction with models able to estimate the inventory for a building based on known parameters or attributes described in the early design phases.

2.7 RESEARCH SPONSORS AND PARTNERS

The Portland Cement Association and the Ready Mix Concrete Research & Education Foundation provided an excellent support to the research at the Concrete Sustainability Hub (CSHub), as well as the Compagnia di San Paolo that financed the MITOR project sponsorship.

3 PROBABILISTIC TRIAGE

As stated in the previous chapter, LCA is often considered cumbersome in the residential building sector, primarily because of the complexity of the data collection required. One way to speed up this process is to apply a *probabilistic triage* to a specific building typology to identify which specific parameters of influence of the building to direct more effort towards in the specification of proxy data in the LCA model.

In the present work, another method to streamline LCA for buildings is proposed based on the probabilistic underspecification approach. With this approach, a system can be characterized according to the available information about its characteristics rather than by specific process-based data (Reis 2013; Olivetti et al. 2013). This approach quantifies environmental results processed with uncertainty analysis, demonstrating that LCA can be applied not only when complete and detailed system specifications are available but also when decisions have to be made in a situation of data exiguity. In particular, a probabilistic triage was developed for different residential building typologies to effectively triage data collection, i.e., to understand which specific parameters of influence of the building to direct more effort towards in the specification during the LCI phase.

3.1 RESEARCH QUESTION

The building sector is considered to be the area with the most potential to deliver long-term and cost-effective greenhouse gas reductions, so the need to minimize the environmental impact in this context is urgent. Recent studies have emphasized that the operational use phase is not the only phase responsible for air emissions and pollution, as the embodied phase represents a significant proportion of total energy and is growing with the emergence of more energy-efficient buildings. Therefore, a methodology such as LCA becomes crucial for sustainable development in the building sector. However, the complexity of data collection and scope definition limits LCA applications. Even if the inventory analysis data have already been collected, tabulated, and indexed, the methodology is still time-consuming, which discourages designers. The main question that this section addresses is whether applying the probabilistic triage approach may provide the ability to understand which components contribute the most to total environmental impacts and therefore how to prioritize data collection and specification.

3.2 METHODOLOGY

This study investigates whether LCA of buildings can be robustly streamlined with an effective and efficient data collection triage and a consequent selected use of surrogate data. Surrogate data consists of less accurate data which could streamline the analysis. However, during the LCI phase, it could also lead to a potential high uncertainty in final results, if not managed adequately. Olivetti et al. published a work in which the bill of activities or the bill of materials associated with the life cycle of a system can be prioritized through probabilistic triage (Olivetti et al. 2013).

Based on this method, the work presented here uses the probabilistic underspecification approach to identify a “high-priority” subset of activities called Set of Interest (SOI) and a “low-priority” dataset that can be characterized with low-fidelity categories. For a given system, the SOI is identified with a statistical simulation and represents the target for a higher resolution. The methodology is described in detail below.

3.2.1 Adapting probabilistic underspecification

The typical procedure for LCA studies conducted with a commercial software is to associate each activity (materials use, energy consumption, emissions, etc.) of the BOA to a specific LCA dataset available in a database. On the other hand, with probabilistic underspecification an LCI can be generalized using low-fidelity categories instead of proxy data or specific LCA datasets for each activity. The probabilistic underspecification approach consists of using structured (and nested) groups of LCA datasets during the LCI phase, in order to obtain distributions of environmental impacts for each system, at different levels of specificity. Several LCA databases (EcoInvent, USLCI, Athena Sustainable Materials Institute, PE International) were explored and available LCA datasets were organized using a hierarchical categorization scheme.

The classification scheme was again developed using the MasterFormat® structure defined by the Construction Specifications Institute (CSI) (Construction Specifications Institute 2014). MasterFormat® lists different main divisions and nested sub-divisions, providing a structured hierarchy for the activities connected to the construction of a building. For this part of the work, each LCA dataset related to construction materials was classified and organized into four hierarchical levels of specificity, instead of five. Level 1 (M1) refers to the less specified category, while Level 4 (M4) identifies the most detailed category, including single LCA datasets available in LCA databases. This decision was taken in order to simplify the classification structure developed in the previous chapter. Moreover, experiments were conducted using the extremes of the classification (M1 and M4).

3.2.2 Probabilistic triage

Through probabilistic triage an SOI can be identified using a statistical ranking system based on the probability that the life cycle activity contributes to some threshold of the total impact of the product. The SOI is defined as the smallest subset of activities whose impact represents a fraction, *T*, of the total environmental impact, *EI*, of the system evaluated at a particular level of specificity (Olivetti et al. 2013). Afterwards, a life cycle analyst can refine the data collection for prioritized targets only, in which components are specified with more detail. This represents a way to streamline the study and therefore to obtain streamlined LCA results. Formally, the SOI for a specific level of detail (M1-M4) is defined as the minimum subset of activities that satisfies equation (3.1):

$$SOI \subseteq \sum | P\left\{\frac{EI_{SOI}}{EI_{TOT}} \geq T\right\} \geq C \tag{3.1}$$

In Equation (3.1) *P* identifies a probability density function and *C* an interval of confidence. EI_{SOI} is the environmental impact due only to the activities of the SOI and EI_{TOT} is the total environmental impact of the system. The values of *T* and *C* can vary and generally depend on the target of the research. For this work, *T* was initially set as 75% and *C* as 90%.

3.2.3 System boundary for case studies

A cradle-to-gate system boundary was applied to the case studies to test this work. In other words the materials used for the initial construction of a series of buildings were used, while other activities (operational use phase, maintenance and replacement, end of life) will be considered in future works. This decision was made in order to limit the scope of the analysis for tests and to facilitate the results interpretation phase. This decision reflected recent work which showed the growing significance of embodied energy inherent in buildings and have demonstrated its relationship to carbon emissions (Dixit et al. 2012). Recent studies have also further emphasized the significance of embodied phase and have acknowledged its relative proportion of total energy, which is growing with the emergence of more energy efficient buildings (Frey 2008; Plank 2008).

3.2.4 Assessment method

The Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) version 2.1, adopted in the previous chapter, was used to calculate the potential environmental impacts, including impact categories such as global warming (CO_2 equivalent), acidification (SO_2 equivalent), eutrophication (N equivalent) and tropospheric ozone (smog) formation (O_3 equivalent).

3.2.5 Evaluation metrics

The median absolute deviation coefficient of variation (MAD-COV) was used as the performance index (see section 2.4.1). In equation (3.2), MAD-COV for a generic environmental indicator and a defined level of specificity (Mj, j = 1:4 and Hybrid) is obtained using each single environmental result of a Monte Carlo simulation (x_i, i = 1:1000) and the median value of all the 1000 Monte Carlo simulation results (median(X_{Mj})). This performance metric was chosen in order to calculate the dispersion in results for each case study and therefore to evaluate the different dispersions occurring with different levels of specificity in order to estimate the effectiveness of hybrid models.

$$MAD - COV_{Mj} = \frac{median(\left|x_{iMj} - median(X_{Mj})\right|)}{median(X_{Mj})} \tag{3.2}$$

On the other hand, the efficiency of hybrid models was evaluated calculating the amount of components in the SOI and the corresponding share of the total BOM.

3.3 CASE STUDIES

The method described in section 3.2 was applied to two classes of existing benchmark buildings, described by Ochsendorf et al. and selected among representations of residential and commercial buildings that the U.S. Department of Energy and its national laboratories have prepared precisely for benchmarking studies. A 2400 ft^2 (223 m^2) two-story single family house and a 33763 ft^2 (3137 m^2) four-story multifamily building. Buildings and their BOMs (list of materials used for the envelope and for internal assemblies) were analyzed for two different climates (Phoenix and Chicago, USA) and for different structural materials (insulated concrete form and light-frame wood house). The buildings were designed in accordance with applicable building codes as well as standard industry practice (Ochsendorf 2011).

The benchmark single-family house considered was modeled for two different climate regions, therefore the Phoenix house is supported by a slab-on-grade foundations while the Chicago house has a basement wall foundation. The main difference between the insulated concrete form (ICF) house and the wood frame house is represented by exterior walls, while the roof, partitions and floors are designed in the same manner. The light-frame wood house in Chicago uses 2x6 in (38 mm x 140 mm) studs at 24 in (61 cm) on center, while the Phoenix wood house uses 2x4 in (38 mm x 89 mm) studs at 16 in (41 cm) on center. The ICF house consists of a 6 in (152 mm) load bearing reinforced concrete wall with 2.5 in (63.5 mm) thick expanded polystyrene (EPS) panels on each side. The exterior cladding is stucco with a metal lath for support and expansion joints. The exterior has three layers of silicate emulsion paint (Ochsendorf 2011).

The benchmark multi-family building consists of a four-story construction for a total of eight apartment units per floor. Again, the main difference between the ICF building and the wood frame building is represented by exterior walls. The ICF structure consists of 8 in (203 mm) load-bearing concrete walls with 2.5 in (64 mm) of expanded polystyrene (EPS) insulation on either side as the formwork. The exterior walls for wood multi-family buildings use 2x4 in (38 mm x 89 mm) studs at 16 in (41 cm) on center, except for the first two levels of the 56 ft (17 m) sides which have 3x4 in (64 mm x 89 mm) studs at 16 in (41 cm) on center. All buildings have a 4 in (10.2 cm) concrete slab-on-grade with a plastic vapor barrier, a 4 in (102 mm) layer of gravel, and a 2 in (51 mm) layer of sand. Additionally, there is a continuous perimeter footing and 5x5 ft (1.5 m x 1.5 m) isolated footings for each column. The exterior cladding is stucco, that utilizes a metal lath for support and expansion joints, and finally three layers of silicate emulsion paint (Ochsendorf 2011).

Complete BOMs for 8 case studies are available in Table 3.1 and Table 3.2.

3.3.1 Single-family detached houses

Table 3.1 - Bill of materials for single-family buildings. Materials for initial construction are reported for two different climate regions (Chicago and Phoenix, USA) and two different construction techniques (Insulated concrete forms, ICF or wood frame). Values in kg, totals may not agree because of rounding.

Values in kg	ICF - Chicago	Wood - Chicago	ICF - Phoenix	Wood - Phoenix
Foundation	**121764.33**	**118364.79**	**80361.00**	**77672.00**
Concrete for perimeter footings	10867.68	8280.14	15788.85	13200.85
Concrete for walls	48128.28	48128.28	9315.15	9315.15
Concrete for slab on grade	26363.64	26363.64	26363.64	26363.64
Concrete for isolated footings	6586.37	6586.37		
Gravel for slab on grade	28636.36	28636.36	28636.36	28636.36
Steel	244.00	244.00	60.00	60.00
Polyethylene film	96.00	96.00	96.00	96.00
EPS Insulation	489.00		61.00	
XPS insulation slab on grade	30.00	30.00		
Plastic ties	323.00		40.00	
Floors	**7105.07**	**6728.99**	**6626.54**	**6296.39**
Wood	2250.15	1897.78	2002.98	1696.54
Plywood	2675.94	2675.94	2675.94	2675.94
Wood Columns	133.64	133.64	133.64	133.64
Insulation over Unheated Basement	231.36	231.36		
Drywall	1746.00	1746.00	1746.00	1746.00
Steel for Connections	67.99	44.27	67.99	44.27
Exterior Walls	**69557.02**	**7596.39**	**69557.02**	**6167.39**
Concrete for walls	67265.41		67265.41	
Steel rebar	541.63		541.63	
Wood for exterior walls		4781.35		3493.15
Plywood for exterior walls		251.65		183.85
Plastic ties	692.00		692.00	
EPS Insulation	1046.00		1046.00	
Fiberglass insulation exterior walls		195.00		122.00
Plywood sheathing		2331.12		2331.12
Steel for connections	11.98	37.26	11.98	37.26
Interior Walls	**3844.81**	**3844.81**	**3702.18**	**3702.18**
Wood for load bearing partitions	1094.32	1094.32	951.68	951.68
Plywood for load bearing partitions	26.84	26.84	26.84	26.84
Paint	88.00	88.00	88.00	88.00
Fiberglass insulation	78.55	78.55	78.55	78.55
Drywall	2557.11	2557.11	2557.11	2557.11
Openings	**1104.00**	**1104.00**	**1104.00**	**1104.00**
Aluminum frame	99.00	99.00	99.00	99.00
Glass	883.00	883.00	883.00	883.00
PVC Expansion	122.00	122.00	122.00	122.00
Cladding walls	**2242.00**	**2242.00**	**2242.00**	**2242.00**
Stucco	2013.00	2013.00	2013.00	2013.00
Paint	51.00	51.00	51.00	51.00
Steel Lath	178.00	178.00	178.00	178.00
Roofing	**8725.16**	**8725.16**	**8347.63**	**8347.63**
Wood	2926.43	2926.43	2548.90	2548.90
Plywood	1113.64	1113.64	1113.64	1113.64
Insulation	318.03	318.03	318.03	318.03
Steel Connections	15.32	15.32	15.32	15.32
Drywall	1708.75	1708.75	1708.75	1708.75
Asphalt	2643.00	2643.00	2643.00	2643.00
Staircase	**490.72**	**490.72**	**490.72**	**490.72**
Plywood	8.21	8.21	8.21	8.21
Laminated Veneer Lumber	209.20	209.20	209.20	209.20
Lumber Wood	273.31	273.31	273.31	273.31

3.3.2 Multi-family residential buildings

Table 3.2 - Bill of materials for multi-family buildings. Materials for initial construction are reported for two different climate regions (Chicago and Phoenix, USA) and two different construction techniques (Insulated concrete forms, ICF or wood frame). Values in kg, totals may not agree because of rounding.

Values in kg	ICF - Chicago	Wood - Chicago	ICF - Phoenix	Wood - Phoenix
Foundations	**704055.17**	**666834.62**	**654138.95**	**511139.73**
Concrete for footings	225089.96	185547.00	179166.80	41494.86
Steel reinforcement for footings	19573.04	15278.00	15579.72	3635.50
Concrete for isolated footings	70012.02	70012.02	70012.02	70012.02
Steel for isolated footings	1033.51	1033.51	1033.51	1033.51
Concrete for slab on grade	186401.11	189058.56	186401.11	189058.56
Gravel	136114.40	138054.93	136114.40	138054.93
XPS	299.74	590.25	300.00	590.00
Polyethylene Film	224.57	227.77	224.57	227.77
Steel rebar	5293.34	5368.80	5293.34	5368.80
Sand	60013.49	60870.78	60013.49	60870.78
Wood		793.00		793.00
Floors	**71628.37**	**71628.90**	**71628.37**	**71628.90**
Wood	24988.56	24988.78	24988.56	24988.78
Plywood	37482.85	37483.16	37482.85	37483.16
Rubber pad	6604.49	6604.49	6604.49	6604.49
Carpet	2552.46	2552.46	2552.46	2552.46
Exterior Wall	**815112.56**	**24397.46**	**792749.47**	**24527.16**
Concrete	786063.77		764303.30	
Steel rebar	14317.64		14109.93	
Plastic ties	9185.88		8930.63	
EPS insulation	5545.26		5405.61	
Fiberglass insulation		1048.40		1048.40
Wood		23349.07		23478.77
Plywood		1228.90		1235.72
Load Bearing Partition Walls	**100618.89**	**100618.89**	**100618.89**	**100618.89**
Wood	11926.13	11926.13	11926.13	11926.13
Plywood	627.69	627.69	627.69	627.69
Insulation	1441.16	1441.16	1441.16	1441.16
Drywall	81427.37	81427.37	81427.37	81427.37
Paint	5196.53	5196.53	5196.53	5196.53
Openings	**11276.11**	**11270.86**	**11280.42**	**11272.58**
Aluminum frames	1234.11	1234.11	1234.11	1234.11
Glass	8183.12	8183.12	8183.12	8183.12
PVC expansion joints	369.49	364.25	373.81	365.96
Interior wood doors	1270.20	1270.20	1270.20	1270.20
Exterior steel doors	219.18	219.18	219.18	219.18
Cladding walls	**92496.74**	**90713.34**	**93396.39**	**91338.36**
Paint	1088.71	1062.00	1102.29	1071.68
Stucco	68837.03	67161.00	69695.66	67760.27
Steel lath	1508.17	1438.00	1526.98	1450.64
Roofing	**49415.67**	**49468.86**	**49542.38**	**49677.07**
Asphalt	6312.95	6312.95	6455.79	6455.79
Gravel	19444.91	19444.91	19444.91	19444.90
Insulation batt	1878.90	1863.00	1862.76	1862.76
Wood	15050.94	15178.10	15050.94	15243.83
Plywood	6450.40	6504.90	6450.40	6533.07
Galvanized Steel	277.57	165.00	277.57	136.72
Staircase	**3218.00**	**3218.00**	**3512.03**	**3512.03**
Wood	1769.90	1769.90	1931.61	1931.62
Laminated Veneer Lumber	1383.74	1383.74	1510.17	1510.17
Plywood	64.36	64.36	70.24	70.24
Elevator Core	**55466.79**	**55466.79**	**55466.79**	**55466.79**
Concrete	51029.44	51029.44	51029.44	51029.44
Steel	4437.34	4437.34	4437.34	4437.34
Columns	**7652.03**	**7915.87**	**7652.03**	**7915.87**
Wood	7652.03	7915.87	7652.03	7915.87

3.4 RESULTS

The buildings described in section 3.3 were used to test probabilistic underspecification and probabilistic triage. The first approach was developed with 4 levels of specificity, from M1 (low-fidelity) to M4 (high-fidelity), while triage was defined through hybrid models of M1 and M4 categories, with the latter category used just for the SOI. Sets of Interest were calculated at Level 1 (M1) as a fraction of cumulative percent impact (T = 75%) with 90% confidence. The ICF single-family detached house located in Chicago (ICF-Chicago) was chosen to show an example of result distributions (for acidification, global warming, eutrophication, smog creation) at different levels of specificity, obtained with Monte Carlo simulations and the procedure detailed in the methodology section.

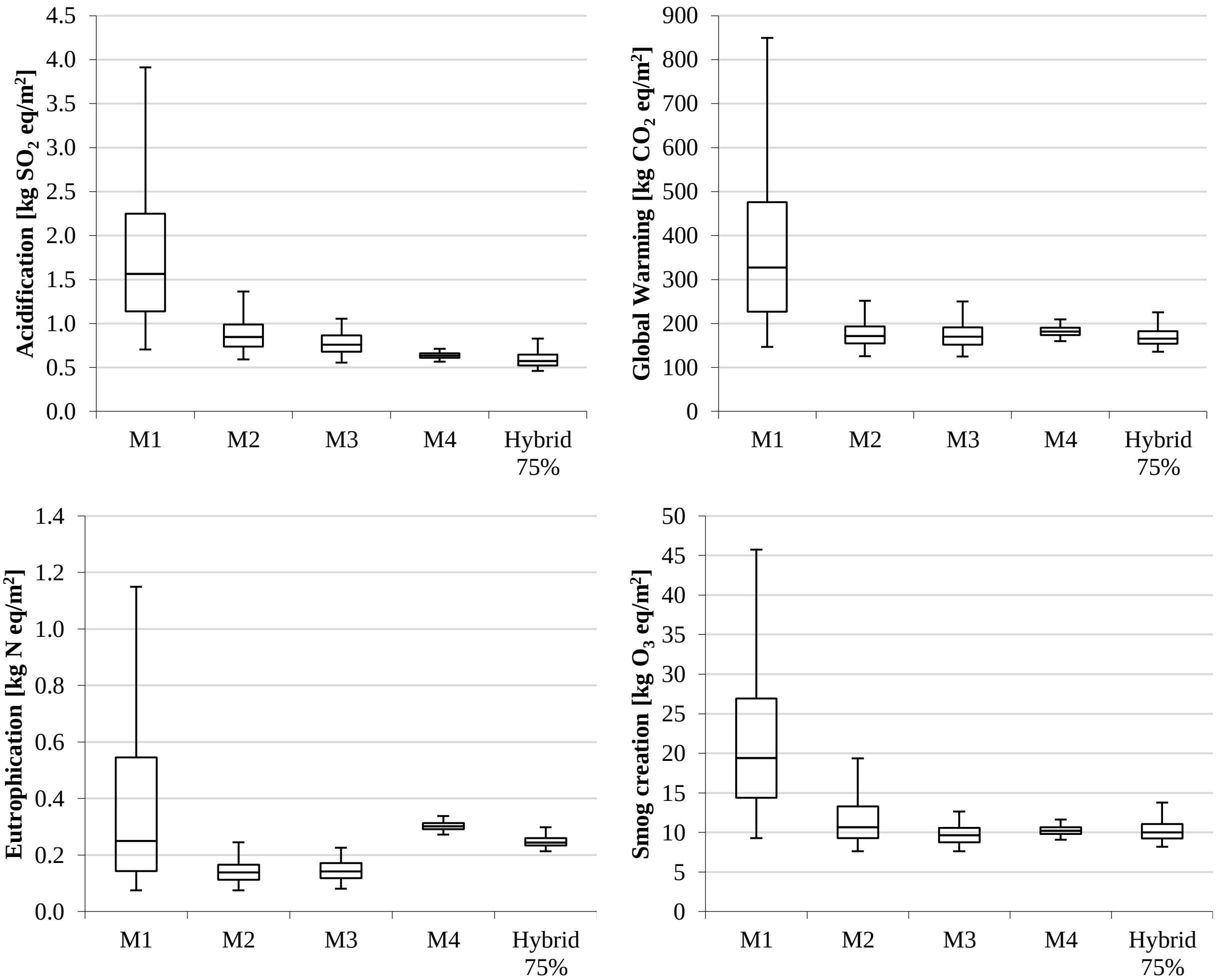


Figure 3.1 - Probabilistic distributions of acidification, global warming, eutrophication, smog creation for the ICF-Chicago single-family house case study. Typical results from an LCA study are represented by M4; the probabilistic underspecification approach is used from M3 to M1, the probabilistic triage is used for hybrid models.

In Figure 3.1 boxplots show the first and third quartiles (25^{th} and 75^{th} percentiles), the band inside the box is the median (50^{th} percentile) and the whiskers represent the 5^{th} percentile and the 95^{th} percentile. Results were normalized to the usable area and therefore referred to 1 m^2.

ICF-Chicago comprises 41 components for a total weight of approximately 215 tons. At M1, the materials of the building were characterized using the broadest groups, such as concrete, metals, thermal and moisture protection, wood plastics and composites, etc. The SOI_{M1} included the components that contribute to 75% of total environmental impacts, with 90% confidence. It is represented by 15 components for acidification (AP), 14 components for global warming (GW), 22 components for eutrophication (EP) and 15 components for smog creation (SM), 40% of the BOM on average. $MAD\text{-}COV_{Hybrid}$ was 7.8% on average when these components were specified at Level 4 (triaged hybrid model), while at Level 1 and Level 4 these values were respectively 37.7% ($MAD\text{-}COV_{M1}$) and 4.2% ($MAD\text{-}COV_{M4}$).

Figure 3.2 and Figure 3.3 show MAD-COV values for the four considered environmental indicators, with scenarios from M1 to hybrid model for single-family detached houses and multi-family buildings. Moreover, these two charts provide information about effectiveness for the eight case studies analyzed using hybrid models.

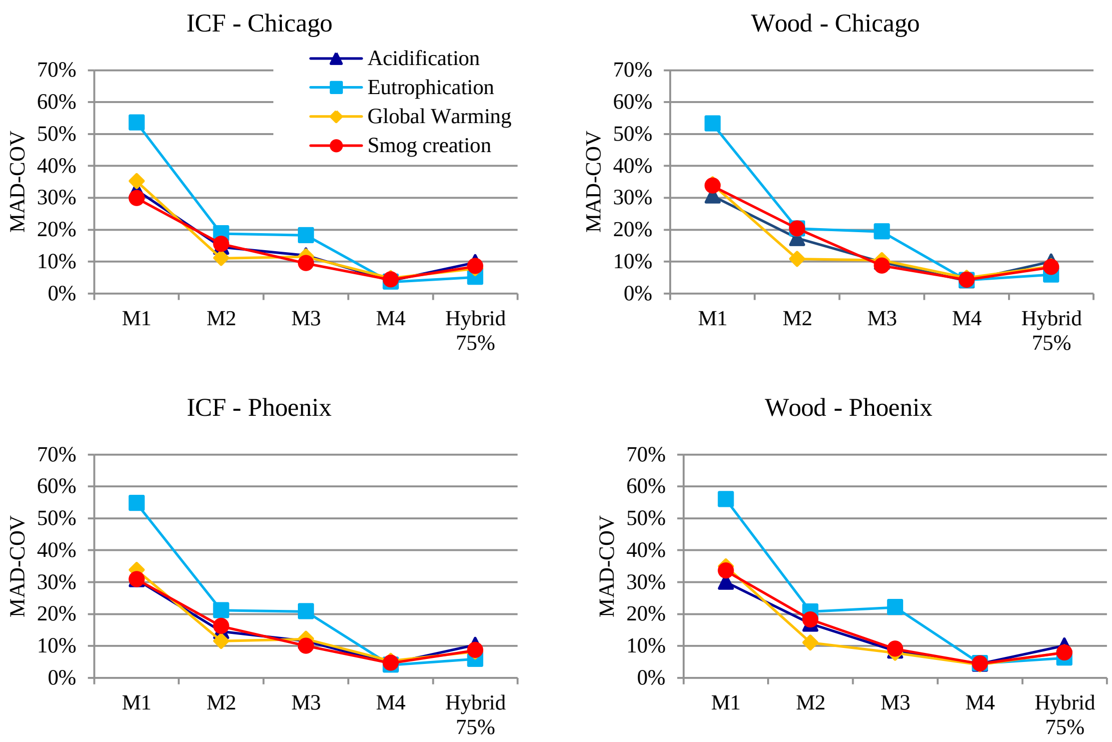


Figure 3.2 - MAD-COV for different environmental indicators at different levels of specification, from M1 to hybrid model (SOI threshold 75%). Single-family detached houses.

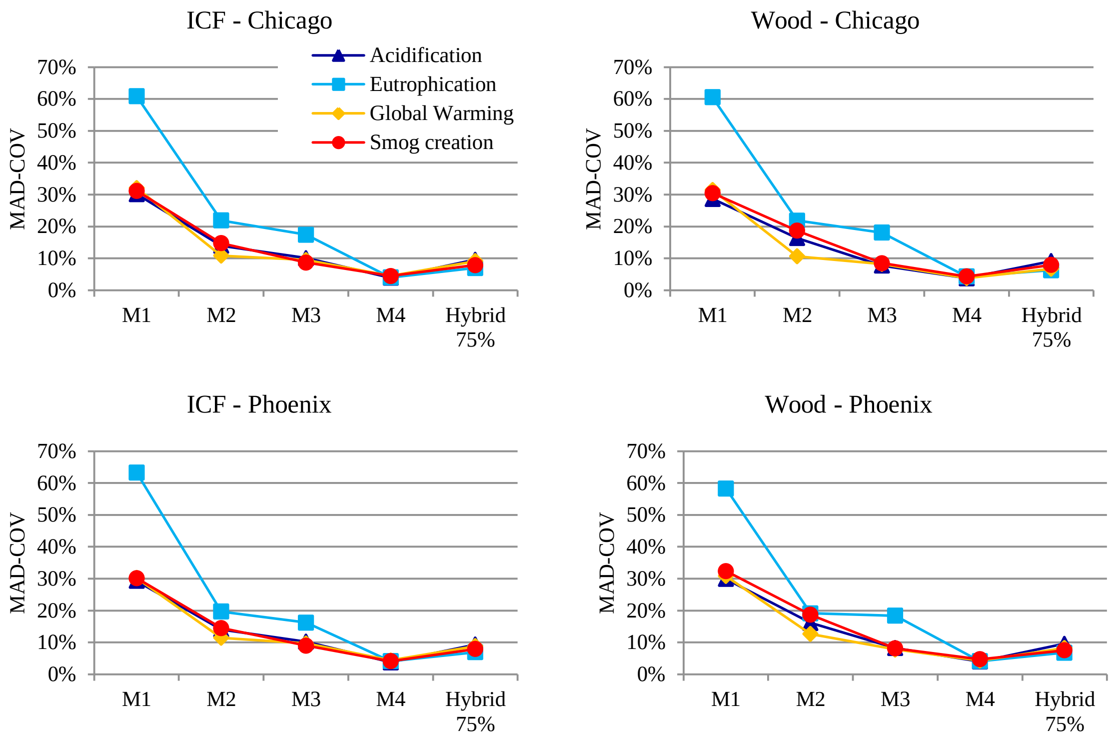


Figure 3.3 - MAD-COV for different environmental indicators at different levels of specification, from M1 to hybrid model (SOI threshold 75%). Multi-family buildings.

3.4.1 Alternative sets of interest

A further test was conducted in order to understand how the SOI changes when the threshold *T* is varied. In the benchmark case (*T* = 75%) about 40% of the BOM, on average, is included in the SOI of hybrid models. The resulting size of the SOI is a function of both *T* and *C*, in particular the threshold *T* was analyzed in the range 50-100% (*T* = 100% implies the overall BOM included in the SOI, therefore this case is equivalent to M4). As *T* decreases, the fraction of the BOM included in the SOI decreases as well, reaching a 25% on average when *T* is equal to 50% (Figure 3.4).

MAD-COV_{Hybrid} values ranged depended on the selected threshold *T*, since the number of components specified at M4 changed. Figure 3.5 shows how the performance metric reached best results when 100% of the BOM is specified at M4. However, by specifying only 40% of the BOM (benchmark hybrid model, *T* = 75%) results had only 3.6% more uncertainty. In the most extreme case, 25% of the BOM specified at M4 resulted in an average MAD-COV_{Hybrid} value of 13.4%, with an increase of about 9.2%.

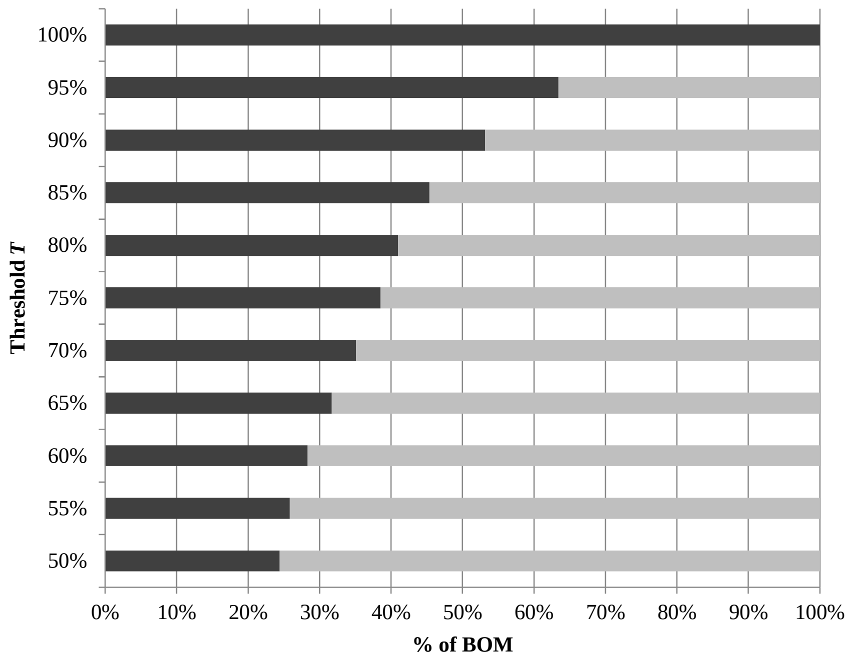


Figure 3.4 - Average fraction of the BOM included in the SOI on varying the threshold T (50 – 100%). ICF-Chicago single-family house case study

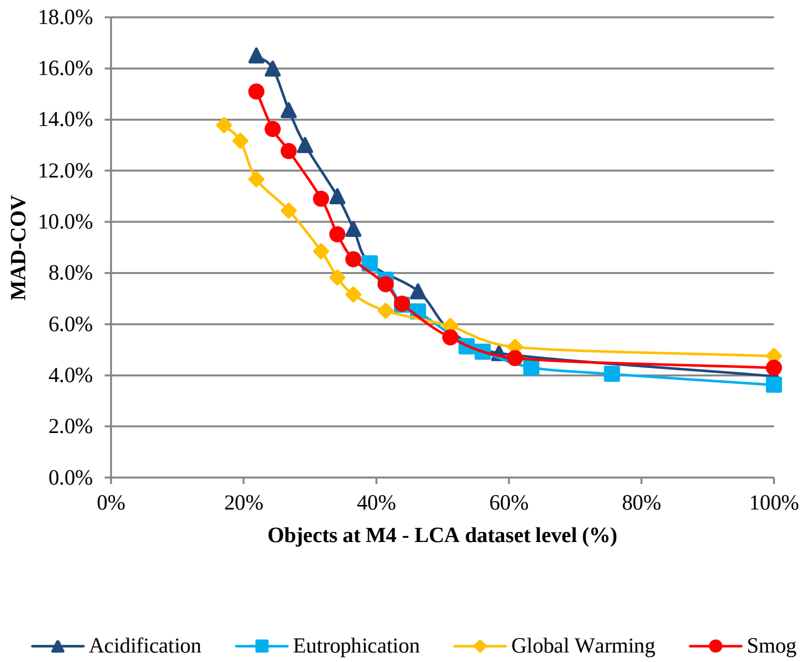


Figure 3.5 - Relation between MAD-COV for hybrid models environmental results and percentage of BOM in the SOI. ICF-Chicago single-family house case study

3.5 Discussion

The purpose of this research was to understand whether probabilistic underspecification and probabilistic triage, as introduced by Olivetti, can streamline LCA studies for the construction sector. Tests were conducted with a series of case studies analyzed with a cradle-to-gate approach, i.e., using the BOM of the construction phase of a building. The aim of these tests was not to compare alternatives (single-family houses versus multi-family buildings, concrete vs. wood frames, humid continental vs. semiarid climate), but to determine if triaged hybrid models can streamline LCA results effectively and efficiently when different building typologies are considered. The effectiveness and efficiency of this method were evaluated by comparing the results obtained to full-fledged LCA results and estimating the reduction in effort during the LCI specification phase.

By using probabilistic underspecification, in this experiment only four classification levels were defined, related to the hierarchical structure of MasterFormat®. For all of the case studies, MAD-COV_{M1} was always higher than 30% on average, while MAD-COV_{M4} resulted generally lower than 5%. Once these results were obtained, probabilistic triage was tested in order to understand how to reduce efforts in specification, thanks to the identification of the activities (i.e., the SOI) that require careful characterization. Concerning the buildings analyzed, triaged hybrid models showed both an effective and efficient way to streamline LCA results. In other words, by specifying only one part of the BOM to the highest level of specificity (i.e., by using individual LCA datasets) results revealed a reduced increase of uncertainty. In benchmark hybrid models, when the SOI was set at threshold T = 75% and confidence C = 90%, single-family houses required 40-44% of the BOM specified with individual LCA datasets, while multi-family buildings required 43-46% of the BOM. This is a potential effort reduction for a resource intensive operation, such as data collection and specification during the LCI phase. Moreover, triaged hybrid models originated MAD-COV_{Hybrid} values ranging from 7.8% to 8.2% for single-family houses and from 7.5% to 8.4% for multi-family buildings, with an increase of uncertainty calculated to be just 4.2% in the worst case.

Finally, hybrid model result distributions proved to be reasonably accurate and obtainable with a reduced need for data specification. However, one can argue about the effectiveness of these results when T is set at 75%, since accuracy is a concept that each analyst can interpret personally and it also depends on the goals of a given LCA study. Therefore several threshold T values were explored, in order to provide an example of result distributions when the SOI is greater or smaller than the baseline case. Using the ICF-Chicago single-family house, different sets of interest were explored whose impacts represented 50% to 100% of total impacts. The lowest limit, T = 50%, introduced a MAD-COV_{Hybrid} of 13.4%, on average, by including 25% of the BOM in the SOI. The threshold T = 60% included 29% of the BOM in the SOI for a MAD-COV_{Hybrid} of 12%. When T was increased to 85%, 47% of the BOM needed the highest specificity and MAD-COV_{Hybrid} became 6.4%. T equal to 95% could represent the best case if accuracy in results is the target: 64%

of the BOM was included in the SOI, MAD-COV_{Hybrid} was 4.7% and the difference with the M4 scenario was negligible (about 0.5%).

Applying probabilistic triage to the BOM of a building made it possible to understand which components contribute the most to its total environmental impact. In detail, for the baseline triaged hybrid models that were analyzed, a recurring set of interest components can be identified. For ICF buildings, the concrete used in exterior walls and foundations played a key role and was always present in the SOI for both single-family and multi-family buildings. For wood frame buildings, given the relatively reduced impact of wood, the main contributors to the SOI were the concrete used for the foundation, the glass used for openings, and the gypsum boards used for interior and exterior walls.

The main motivation for the tests conducted in this work was to understand whether probabilistic triage can be used to streamline the LCA of buildings by prioritizing data collection and specification. Here, the probabilistic underspecification data are gathered and described using basic categories and therefore, an analysis can begin with a very rough estimate of impact. However, probabilistic triage is aimed at understanding and forecasting the specific parameters of influence for a system (materials, assemblies, activities, etc.), which stress the specification during the LCI modeling phase. This introduces a potential reduction of the issues and bias caused by the use of surrogate data or inappropriate LCA datasets during the LCI phase.

In future works, probabilistic triage will be tested considering the overall life cycle of a building (including the operational use phase and end of life) and not only its initial construction. In this way, for a specific building typology and a specific context (location, climate zone, etc.), the parameters and activities of particular importance can be identified. This will potentially allow a life cycle analyst to know where to focus attention and concentrate data collection and specification efforts, thereby reducing the time and costs associated with long-established full-fledged LCA studies.

The case studies considered were characterized by a complete list of measured materials, so an important area of future work would be uncertainty in quantities of materials used for a given building typology. Therefore, further research is needed to forecast the materials requirement of a residential building before construction (or during the design phase).

Regarding probabilistic underspecification, four levels of specificity were used, but this decision was arbitrary and other structures could be analyzed depending on the goals of the LCA study. A recent study introduced the use of data mining to develop a material taxonomy, but further work is needed to determine the most appropriate classifiers as well as what classifier information would be most easily available to final users (designers, architects, scientists, engineers, etc.)

Finally, probabilistic triage was tested using the extreme levels of the classification (M1 and M4), but this was again an arbitrary decision. Future works will explore the possibility of using flexible hybrid models (M1 or M2 or M3 and M4) that can be used in different stages of the design process. By taking into account the experience of professionals (architects and designers), streamlined LCA methods can be developed to support decisions made during the design process.

4 EX-ANTE LCA APPROACH

The application of fully-fledged LCA to innovative materials presents two major limitations: it can be performed primarily as an *ex-post* analysis (i.e., after the industrial production of the new material) and it does not account for the intrinsic properties of the material. To overcome such limitations and forecast the potential impact of a product before its large-scale production, a radical change in perspective is warranted: a shift from an *ex-post* approach to an *ex-ante* analysis (Roes and Patel 2011). In the present work, a comprehensive and straightforward assessment approach (scale-up protocol) is proposed, which is aimed at assessing the environmental sustainability and economic feasibility of the introduction of a new material onto the market before it is produced at an industrial scale.

4.1 RESEARCH QUESTION

Polybutylene succinate (PBS) is an aliphatic polyester proposed as an alternative polymer for the production of polymeric films, among other possible uses. Industrial productions of PBS granules exist, but those are primarily focused on the fossil-fuel-based polymer, and just a few production processes use bio-based input materials (Ichikawa and Mizukoshi 2012). PBS can be partially produced by renewable sources, in particular the bio-based succinic acid, one of the starting monomers. Laboratory-scale productions are possible, but the complete industrialization of the manufacturing process in Europe may take a relatively long time, and so the primary data collection required for a full LCA study is not possible. The research question is related to the environmental burden of the future production of partly bio-based PBS in Europe: is it possible to forecast the environmental burden of an innovative material without optimized primary data? An ex-ante LCA approach is needed to answer this question. Furthermore, this approach should satisfy the following criteria:

- Rely on primary data obtained from simple chemical models and pilot productions;
- Be relatively easy to apply by considering the efficiencies of the best available technologies (BAT) of similar existing technologies;
- Include an uncertainty analysis in order to produce robust distributions of results.

4.2 BIO-BASED POLYMERS

Interest in bio-based plastics as substitution materials for petroleum-based plastics has increased in recent years. In particular, the annual growth rate of the bio-based plastics market between 2003 and 2007 averaged 40% worldwide (Shen et al. 2010) and global industrial plastic production is expected to experience 400% growth by 2017 (European Bioplastics 2013) reaching a total production of approximately 3.45 Mt in 2020 (Shen et al. 2009). This growth is due to a market demand for products with a lower environmental burden compared to traditional plastics and that are not dependent on fossil fuels. From a technological perspective, Shen et al. estimated the maximum technical substitution potential of bio-based polymers by interviewing industrial experts and stated that the replacement of oil-based plastics by bio-based polymers may reach 90% of total global plastic consumption, not considering resource availability or economic constraints (Shen et al. 2010). Thus, the need to quantify biopolymers' environmental impacts is becoming more important due to the requirement to provide a concrete and objective answer to the market.

In most cases, LCA studies of bio-based polymers have produced favorable results with respect to oil-based alternatives, but those evaluations have been subject to the initial assumptions and boundaries of the system considered (Madival et al. 2009). Additionally, a relatively lower environmental burden does not imply the full sustainability of the bio-based plastics currently on the market (Álvarez-Chávez et al. 2012).

A part from starch-based plastics and polylactic acid (PLA), many biopolymer production technologies are still at the lab/pilot-plant scale. Therefore, as for most bio-based products, limited reliable primary data are available with which to perform a proper environmental impact assessment by means of LCA (Patel et al. 2012). For this reason, an *ex-ante* LCA approach is here proposed to assess the environmental performance of innovative bio-based products, by combining primary data collected at the lab/pilot scale with chemical and thermodynamic considerations.

4.3 METHODOLOGY

The final goal of this work is to integrate *ex-ante* LCA with multi criteria material selection, moving from an evaluation based on the unit of mass of the material to an assessment that takes into account at the same time both the intrinsic properties of the material and its environmental burden. This synergic integration represents the most relevant added value element of the proposed methodology.

4.3.1 Scope definition

A cradle-to-gate system boundary is adopted. The initial phases of the material life cycle are considered, including all of the processes leading to the production of the polymer pellet. A reference unit of 1 kg of partly bio-based PBS is used to guarantee the consistency of results and direct comparability with the ecoprofiles available on the PlasticsEurope platform.

4.3.2 Ex-ante LCA ecoprofile based on uncertainty analysis

The operational framework for an *ex-ante* LCA is defined according to ISO 14040 standards for a full-fledged LCA (ISO 14040 2010; ISO 14044 2010). The *ex-ante* LCA strategy proposed in the present work is grounded in the *Generic Approach*, developed by Patel et al., and it is focused mainly on the analysis of bio-based products (fuels, chemicals and polymers) in the context of *White Biotechnology* (Patel 2006). The

Generic Approach is defined as a method that allows the estimation, *ex- ante*, of the environmental impacts and basic economics of new biotechnological processes for which data from the pilot plant or laboratory scale are not yet available or for which industrial-scale data are not publicly accessible due to confidentiality agreements. Such methodology was implemented utilizing primary data from production at the pilot plant scale and secondary data obtained by means of a stoichiometric model of the chemical processes involved. The aim is to perform a multiscale analysis whose results will be suitable for enabling a consistent scale-up of the environmental burden at the industrial scale.

To ensure the feasibility of the analysis, some conditions have to be granted: (a) the biotechnological processes examined (fermentation, enzymatic conversion, etc.) have to be described in the literature and to be considered feasible; (b) the availability of basic information, theoretical and otherwise (for example, the stoichiometry of chemical reactions involved), is defined; and (c) the products analyzed have to be likely produced in large quantities within the current techno-economic context or in a reasonable future scenario.

The main objective of such an analysis is to evaluate the environmental burden associated with the production of goods and, in particular, to allow a comparison with traditional products of the chemical industry. In this context, the scope of investigation is limited *from cradle to factory gate*: i.e. the system boundaries are chosen so that the final output is the studied chemical product. As far as biopolymers are concerned, the eventual goal is to extend the scope of the change-oriented assessment to include the *use phase* by means of material indices. These indices combine mechanical properties with environmental burdens for a straightforward comparison with the oil-based polymers currently in use. In the case of compostable or biodegradable polymers, appropriate considerations are required and the horizon of the analysis may need to be extended *from cradle to grave*, to include also the potential impacts associated with disposal and waste management (Davis and Song 2006; Song et al. 2009).

Once the goal and scope of the analysis have been defined, subsequent steps of the *ex-ante* LCA include the creation of a *flow chart* representing the product system and describing inputs, outputs and internal mass and energy flows. Such a Life Cycle Inventory analysis is a more time and resources-demanding step, similar to the requirements of a full-fledged LCA. As mentioned above, the *ex-ante* LCA methodology adopted here does not rely on primary data collected by monitoring real industrial systems, as these do not yet exist for the production of interest, but on primary data from the lab/pilot plant scale and on a theoretically grounded model. Such a model is based on the current literature and can use analogous industrial processes, for which quantitative and qualitative information are available as a benchmark. Once the processes involved in the production system have been identified, the total energy consumption and the associated environmental impacts are estimated.

In a full-fledged LCA, manifold impact categories are considered consistent with the chosen level of detail and the quality and quantity of available data. Each category summarizes the environmental effects associated with specific emissions. During the development of the ex-ante LCA approach, the following impact categories were used:

- Cumulative Energy Demand (CED) is one of the major causes of environmental impact and it represents a practical and direct approach because all industrial processes consume energy. It measures the amount of energy involved in a system, considering the upper heating value, from both renewable and non-renewable sources.
- Global Warming (GW) is one of the indicators of greatest importance because it is used as a reference in many regulatory measures and environmental policies at the international level. It takes into account, first and foremost, the emissions of carbon dioxide, and other greenhouse gases such as CH_4, N_2O, etc. In the case of bio-based products, carbon uptake (i.e. the CO_2 absorbed during photosynthetic processes) acquires particular relevance and must be accounted for.

The choice of such a small set of indicators, however, does not affect the validity and comprehensiveness of the analysis. In fact, by linear regression, it is possible to associate total energy consumption (CED) with most impact categories, such as acidification, eutrophication, human toxicity, etc., as shown by Roes and Patel. This correlation has been verified for a large number of products, in particular commodities, and it is justified by the fact that energy consumption (in particular from fossil sources) is the primary source of all impacts associated with their production (Huijbregts et al. 2006; Huijbregts et al. 2010). Nevertheless, CED does not take into account impacts resulting from land use, and for this reason, it cannot be regarded as a comprehensive indicator in the case of agricultural products and/or derivatives (Hellweg et al. 2010; Patel et al. 2012). Therefore, in future works, the assessment of energy-related impact categories with land use and land use change indicators will be implemented.

4.3.3 Scale-up protocol

The scale-up protocol is first presented in general terms and afterwards applied to polybutylene succinate, the bio-based polymer chosen as a case study. To obtain a forecast of the environmental results in a cradle-to-gate framework, this methodology is based on the identification of a proper mathematical relationship between the environmental burdens at the stoichiometric, pilot and industrial scales. This relationship is here called the scale-up function. The protocol is made up of five fundamental steps:

- *(1) Choice of reference polymer*. Because data collected on the industrial scale are not available for innovative bio-based products, the definition of the scale-up function requires the choice of a reference polymer. This is selected according to the following considerations: (a) the reference polymer and the biopolymer should belong to the same polymer class (e.g. polyesters); (b) the synthesis of the reference polymer and of the biopolymer should follow comparable chemical routes; and (c) data on the industrial scale must be available for the reference polymer.

- *(2) Pilot scale production and assessment*. One or more batches of the bio-based polymer are produced in a monitored pilot plant: all of the inputs and outputs of the process and the pilot scale environmental impacts of the biopolymer are determined with the *ex-ante* LCA approach. Afterwards, a batch of the reference polymer is produced in the same pilot plant, again monitoring all of the inputs and outputs of the process, and the pilot scale environmental impacts of the reference polymer are determined with the *ex-ante* LCA approach. In this way, data on the environmental burdens of the biopolymer and the reference polymer are obtained straightforwardly on the same production lab/pilot scale.
- *(3) Industrial scale assessment of the reference polymer*. The environmental impact related to the production of the reference polymer on the industrial scale is assessed, by means of a full-fledged LCA, using available secondary data or product ecoprofiles.
- *(4) Stoichiometric baseline*. For both the bio-based polymer and the reference, it is possible to define stoichiometric models for the chemical conversions (e.g. polymerization) based on theoretical information. These models represent perfectly efficient ideal systems; therefore, their environmental impact (assessed by means of *ex-ante* LCA) is the lowest possible for the production routes considered, so it is used as a baseline.
- *(5) Scale-up function definition*. The result of the previous steps is a set of environmental impact values on the pilot, industrial and stoichiometric scales for the reference polymer, whereas the environmental burden on the industrial scale is still missing for the new biopolymer. Therefore, considering the complete set of data pertaining to the reference polymer, a relationship among the impacts at different scales (Environmental Impact, EI) is defined as function of the mass conversion yield (y_{mass}) of the chemical conversion process.

$$EI_{ref} = f(y_{mass,ref}) \tag{4.1}$$

The mass conversion yield is a valid indicator of the scale of a chemical process: the pilot scale is characterized by high inefficiency and then it has a low y_{mass}: conversely, industrial production is optimized (hypothesis of BAT) and it has a much higher y_{mass}. Finally, the stoichiometric model is representative of the ideal process and y_{mass}^{stoic} represents the upper limit for the conversion. Because the stoichiometric mass conversion yield is characteristic of the specific process considered and it does not depend on factors that are not chemical and physical, the y_{mass} at each scale is normalized with respect to

y_{mass}^{stoic} to enable the subsequent application of the function to slightly different processes. Therefore, equation (4.1) is rewritten as follows:

$$EI_{ref} = f(\bar{y}_{mass,ref}) \tag{4.2}$$

where $\bar{y}_{mass,ref}$ is the normalized mass conversion yield. Equation (4.2) is the generalized form of the *scale-up function*. The set of data for the environmental impact of the reference polymer is made up of discrete points: therefore, a regression or interpolation is required to obtain a proper mathematical function.

4.3.4 Monte Carlo simulations

For this specific work, Monte Carlo analysis was used to process uncertainty data for all of the assessments: this way, for each parameter, there is not only one value representative of the impact, but a range of data points (domain of possible inputs), defined by a probability distribution and the standard deviation. Monte Carlo simulation randomly generates inputs from the probability density function over the domain and performs a deterministic computation on the generated inputs.

The entire simulation was run 1000 times for each assessment to obtain a significant number of trials. Finally, each parameter of the LCA dataset is characterized by a distribution of results; these are then aggregated to obtain the total probabilistic distribution.

4.4 CASE STUDY

The case study addressed herein is focused on polybutylene succinate PBS, a biopolymer that is gaining interest, particularly as a replacement for polyolefins (Fujita and Wada 2011; Jacquel et al. 2011). This biopolymer is partly bio-based (i.e., it can be obtained from bio-based monomers, in particular bio-based succinic acid) as well as biodegradable (it satisfies the criteria of ISO 14855 (ISO 14855 2005)).

PBS is an aliphatic polyester with mechanical properties and processability performances similar to those of widely used polymers. It has been proposed as an alternative in the production of polymeric films for use in agriculture (mulching film), shopping bags, bags for composting, etc. (Ichikawa and Mizukoshi 2012).

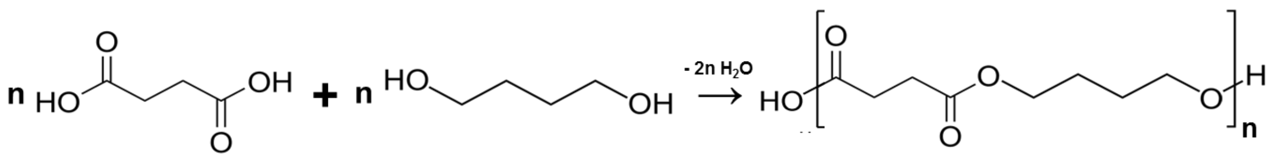


Figure 4.1 - Polybutylene succinate chemical reaction

PBS is obtained from succinic acid and 1,4-butanediol monomers by means of a polycondensation reaction that forms the polyester and water as byproduct (Figure 4.1). Currently, the fossil monomers are, but alternatives from renewable sources have been studied to replace one or both of the reactants. In particular, succinic acid can be produced from starch, glucose or cellulose, through yeast-based or bacterial fermentation with a relevant potential reduction in CO_2 emissions (Smidt et al. 2011). Furthermore, bio-based succinic acid can become the source for a "green" C4 chemical derivatives platform, including 1,4-butanediol (Deshpande et al. 2002; Werpy et al. 2004; Patel 2006; Minh et al. 2010; Jacquel et al. 2011). A sensitivity analysis was performed to evaluate and compare different renewable sources and chemical routes available for the production of bio-based succinic acid. The biomasses considered were maize starch, sugarcane, and lignocellulosics, and the methods of extraction taken into account were crystallization and electrodialysis, for a total of 6 different cases analyzed. Data about the environmental impact of bio-based succinic acid were derived from Patel (Patel 2006).

The Japanese company *Showa Highpolymer* has successfully produced PBS on the pilot scale using bio-based succinic acid. The mechanical properties and processability (extrusion bubble test) of the resulting bio-based PBS are in line with the performance of its oil-based counterpart (Ichikawa and Mizukoshi 2012). Because the production process of PBS from biomass is currently on the pilot scale, a forecast of its environmental impact on an industrial scale holds significant interest.

The starting monomers for the production of PBS are a dicarboxylic acid and a diol undergoing an esterification reaction. According to step 1 of the scale-up protocol, the reference polymer should be a polyester obtained with the same chemical reaction (polycondensation) and for which an industrial ecoprofile is available. From a purely chemical point of view, one of the closest polymers to PBS is polybutylene terephthalate (PBT) because, although it is partly aromatic, it is obtained by polycondensation of terephthalic acid and 1,4-butanediol. Therefore, PBT meets both requirements (a) and (b) for the selection of the reference polymer in the first step of the scale-up protocol, but at present, a trustworthy ecoprofiles for this material is not available. For this reason, it was disregarded and polyethylene terephthalate (PET) was selected as an alternative. PET is produced from terephthalic acid (dicarboxylic acid) and ethylene glycol (diol) by means of polycondensation (Figure 4.2). Furthermore, a comprehensive ecoprofile for PET is available from PlasticsEurope[13]. Thus, PET satisfies all of the selection requirements and is a suitable candidate for use as reference polymer for the scale-up of the environmental impact of PBS.

[13] http://www.plasticseurope.org/

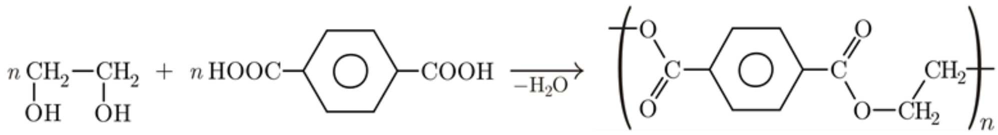


Figure 4.2 - Polyethylene Terephthalate chemical reaction starting from Terephtalic Acid and Ethylen glycol.

4.4.1 Bio-based succinic acid

As reported in the BREW Project report (Patel 2006), Succinic acid (HOOC-CH2-CH2-COOH) is an aliphatic, saturated C4 dicarboxylic acid. It is typically produced by catalytic hydrogenation of petrochemically derived maleic acid or maleic anhydride, but can also be produced fermentatively from carbohydrates in a mixed-acid fermentation.

The methodology and environmental impact results for a bio-based succinic acid production are detailed in the report, considering a functional unit of one ton of organic chemical and the so-called Generic Approach, a method that estimates the environmental impacts of new biotechnological processes for which process data are not publicly available. Bio-based succinic acid can be obtained via anaerobic batch fermentation on dextrose substrate. The starting material (biomass) can be maize starch, sugar cane or lignocellulosics, while the workup can be done via crystallization or electrodialysis, therefore making available six different options and six different environmental impact profiles.

Table 4.1 provides information about total energy use, greenhouse gases emission and land use for the six available options, using a cradle to gate approach.

On the other hand, the EcoInvent process "c1,4-butanediol, at plant, RER" has been used to model the production of 1,4-butanediol from acetylene in Europe. Raw materials, energy consumptions and emissions are modelled with literature data using a process of hydrogenation of butynediol from acetylene.

Table 4.1 - Succinic acid total energy use, greenhouse gases emission and land use for a cradle-to-factory gate basis

	Non renewable energy use GJ/t	Renewable energy use GJ/t	Total energy use GJ/t	Biogenic carbon stored t CO_2 eq/t	Greenhouse gases emission t CO_2 eq/t	Land use ha/t
Bio-based succinic acid Maize starch Crystallization	66.5	36.1	102.6	-1.5	3.1	0.26
Bio-based succinic acid Maize starch Electrodialysis	27	34.7	61.7	-1.5	0.8	0.25
Bio-based succinic acid Sugar cane Crystallization	44.9	63.9	108.8	-1.5	2.1	0.26
Bio-based succinic acid Sugar cane Electrodialysis	5.4	62.5	67.9	-1.5	-0.2	0.26
Bio-based succinic acid Lignocellulosics Crystallization	54.5	49.7	104.2	-1.5	2.5	0.17
Bio-based succinic acid Lignocellulosics Electrodialysis	15	48.2	63.2	-1.5	0.2	0.17

4.4.2 Pilot plant

PBS and PET samples were synthesized via a two-step melt polycondensation reaction using a 7.5-L stainless steel batch reactor equipped with a heating system, a mechanical stirrer with torque measurement, a distillation column, a vacuum line and a nitrogen gas inlet (Jacquel et al. 2011). Chemical processes involved in the reaction are represented in Figure 4.3 and Figure 4.4. Primary data (material inputs/outputs and energy consumption) from pilot plant was collected, initially taking into consideration the phases of boiler ignition and final reactor cleaning, which have been later removed in order to emulate a continuous industrial production process. Details about the primary data collected are available in section 4.4.3.

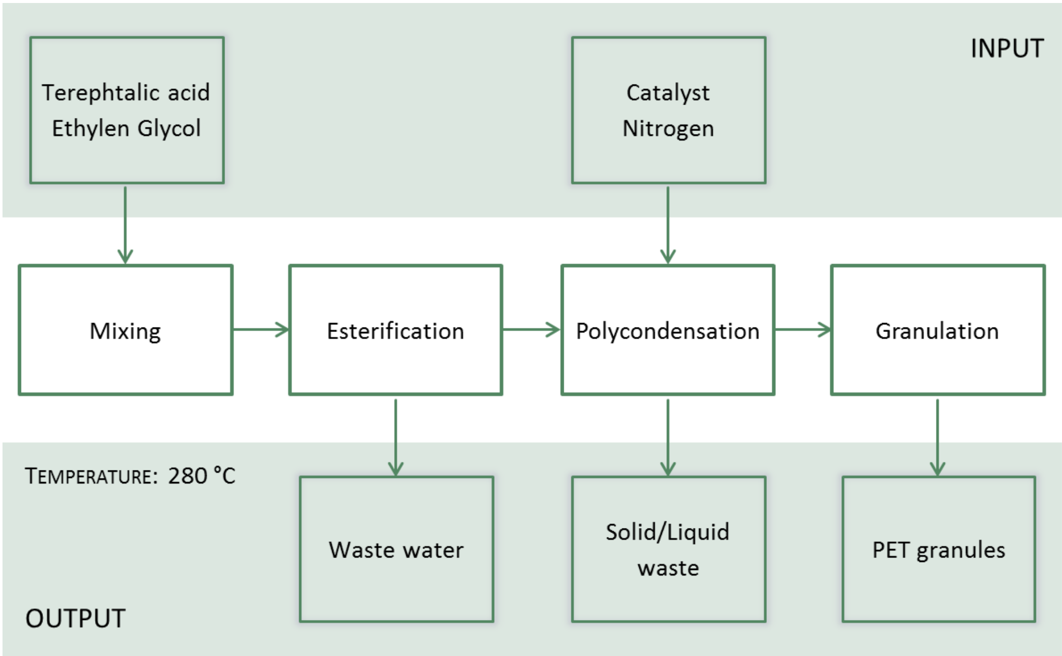


Figure 4.3 - Polybutylene succinate production at pilot plant.

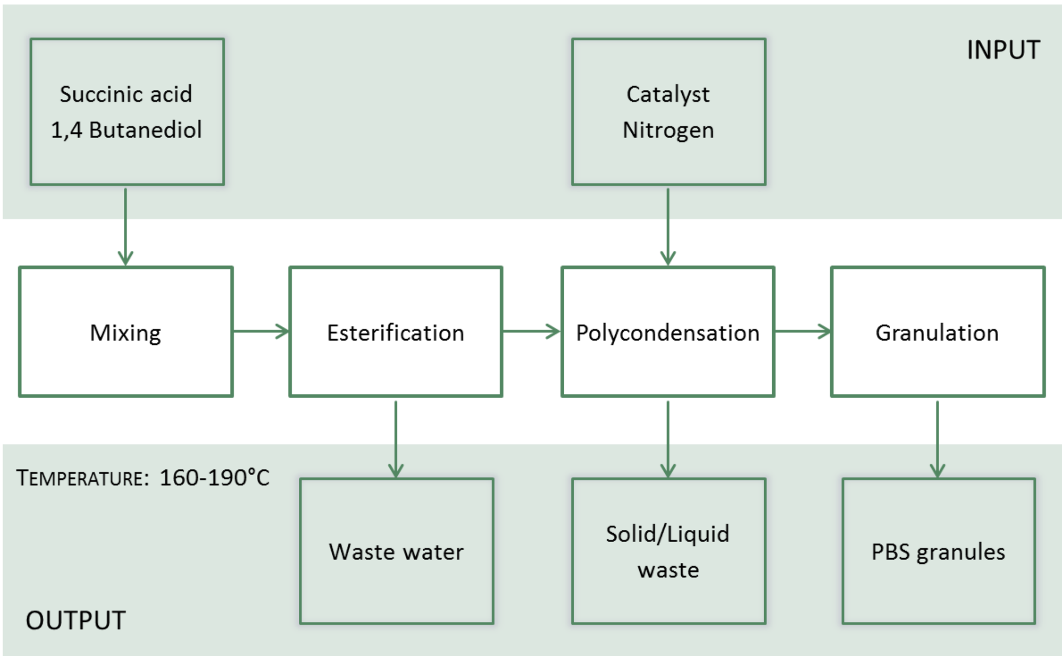


Figure 4.4 - Polyethylene Terephthalate production at pilot plant

4.4.3 Data collection

In accordance with step 2 of the scale-up protocol, some batches of PBS and PET were produced in a pilot plant (Jacquel et al. 2011), while monitoring the process parameters, i.e. the input and output flows of reactants, products, emissions and waste as well as energy consumption. Because a pilot process is characterized by small batch production, there is a power absorption associated with the initial heating of the system and with its final cleaning. The energy related to these phases of the process was neglected to mitigate the effects of the discontinuous nature of pilot production and to approach the operative conditions of a large batch or a continuous system. The primary data (Table 4.2 and Table 4.3) collected were used to determine CED and GW for both the polymers produced on pilot scale.

Table 4.2 - Inventory data for PET on the pilot and stoichiometric scales.

PET	Pilot	Stoic.
Input (kg)		
Terephtalic Acid	2.66	0.87
Ethylene glycol	1.19	0.32
Liquid Nitrogen	10.15	-
Ethylene glycol (for cleaning)	11.13	-
Output (kg)		
PET Pellet	2.60	1.00
Ethylene glycol (unreacted)	0.07	-
Ethylene glycol (for cleaning)	11.13	-
Nitrogen waste	10.15	-
Waste water	0.44	0.19
Energy consumption (MJ)	220.54	0.85

Table 4.3 - Inventory data for PBS on the pilot and stoichiometric scales.

PBS	Pilot	Stoic.
Input (kg)		
Succinic Acid	1.89	0.69
1,4-Butanediol	1.51	0.52
Liquid Nitrogen	10.15	-
Ethylene glycol (for cleaning)	11.13	-
Output (kg)		
PBS Pellet	2.10	1.00
1,4-Butanediol (unreacted)	0.07	-
Ethylene glycol (for cleaning)	11.13	-
Nitrogen waste	10.15	-
Waste water	0.44	0.21
Energy consumption (MJ)	198.37	0.95

Afterwards, following step 3 of the protocol, the impact for PET on the industrial scale was assessed with secondary data (*Polyethylene terephthalate, granulate, amorphous, at plant/RER U*, as implemented in SimaPro).

Finally, the inventory data used to determine the stoichiometric baseline (step 4) were obtained from the chemical reactions involved in the polymerization of PET and PBS. In this case, energy consumption was estimated according to the polycondensation enthalpy of reaction, computed by means of Hess's law. These "theoretical" inventory data (Table 4.2 and Table 4.3) were then used to assess the environmental burden (CED and GW) of the ideal stoichiometric scale production.

For steps 2, 3 and 4, the uncertainty of the impact assessment was processed by means of Monte Carlo simulation. This resulted in two sets of data points, for the reference polymer (PET) and for biopolymer (PBS). Each assessment was iterated 1000 times, giving rise to a statistical distribution of results whose most significant values were considered (i.e. the 5th, 25th, 50th, 75th and 95th percentiles). Each data point is defined by the value of the environmental impact (EI) and the corresponding normalized mass conversion yield ($\bar{y}$) that characterizes the scale of production:

$$(EI, \bar{y}) \tag{4.3}$$

4.5 SCALE-UP FUNCTIONS

The last step of the protocol consists of the identification of the scale-up function. Starting from the set of data points of the reference polymer, different mathematical functions (regressive or interpolating) were identified. In particular, linear, logarithmic, polynomial and power regression as well as linear interpolation were analyzed. Afterwards, each of these functions was translated along the ordinate axis to fit with the biopolymer data points.

In the case of regression functions, the industrial point (EI_{ind}) was identified by computing the value of the scale-up function corresponding to the normalized mass conversion yield in the best available technology hypothesis:

$$EI_{ind} = f(\bar{y}_{BAT}) \tag{4.4}$$

The resulting impacts were inconsistent with the stoichiometric limit, and therefore, they were disregarded. On the other hand, linear interpolation proved to be a suitable trade-off between accuracy of results and ease of implementation. For this reason, linear interpolation was adopted in the present work. The minimum subset of data points defining the environmental impact of the reference polymer at different production scales is represented as follows:

$$\{(EI_{pilot}, \bar{y}_{pilot}), (EI_{ind}, \bar{y}_{ind}), (EI_{stoic}, \bar{y}_{stoic})\} \tag{4.5}$$

This subset of points can be obtained by following the scale-up protocol as previously detailed. The linear interpolation on the set defined in (4.5) is represented by the concatenation of the linear interpolants between each pair of data points. The resulting function (general example in Figure 4.5) is continuous of class C^0 and is defined by the following:

$$\begin{cases} \bar{y}_{pilot} \leq \bar{y} \leq \bar{y}_{ind}; \; EI = m' \cdot \bar{y} + c' \\ \bar{y}_{ind} \leq \bar{y} \leq \bar{y}_{stoic}; \; EI = m'' \cdot \bar{y} + c'' \end{cases} \tag{4.6}$$

where m' and m'' are, respectively, the slopes of the lines interpolating the pilot-industrial data points and the industrial-stoichiometric ones. Equation (4.6) is called the *linear scale-up function*, and it can be used straightforwardly to forecast as a first approximation, the potential environmental impact of production of the biopolymer on an industrial scale.

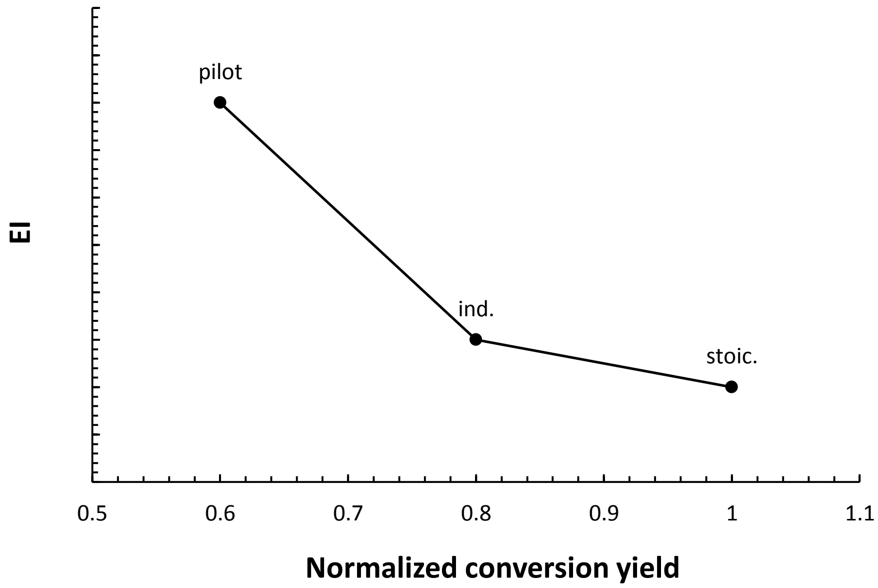


Figure 4.5 - Linear interpolation of reference polymer minimum subset of data points (general example).

According to previously described scale-up protocol, the minimum subset of data points for the biopolymer is as follows:

$$\{(EI_{pilot}, \bar{y}_{pilot}), (EI_{stoic}, \bar{y}_{stoic})\} \quad (4.7)$$

The data point representing the biopolymer impact on the industrial scale is missing, and it can be forecasted by means of the scale-up function defined from the set of data points of the reference polymer. If the reference polymer is chosen properly (first point of the scale-up protocol), it can be assumed that the environmental impact, as a function of the normalized mass conversion yield, has the same trend for both the reference polymer and for the bio-based polymer. Thus, with reference to the scale-up function (4.6), the following can be written:

$$\begin{aligned} m'_{ref} &\cong m'_{bio} \\ m''_{ref} &\cong m''_{bio} \end{aligned} \quad (4.8)$$

In particular, the first part of function (4.6) is considered, relating pilot and industrial scale impacts for the reference polymer and the angular coefficient m', a sheaf of lines for the biopolymer it can be defined:

$$EI_{bio} = m' \cdot \bar{y}_{bio} + c \tag{4.9}$$

Within such sheaf of lines, the line passing through the pilot scale data point can be identified $(EI_{pilot}, \bar{y}_{pilot})$:

$$EI_{bio} = m' \cdot \bar{y}_{bio} + c'_{bio} \tag{4.10}$$

Similarly, taking into account the second part of Equation (4.6), the angular coefficient m'' and the data point $(EI_{stoic}, \bar{y}_{stoic})$, it is possible to identify the line passing through that point:

$$EI_{bio} = m'' \cdot \bar{y}_{bio} + c''_{bio} \tag{4.11}$$

Finally, the intersection of (4.10) and (4.11) determines a point that represents the environmental impact of the bio-based polymer on the industrial scale (Figure 4.6).

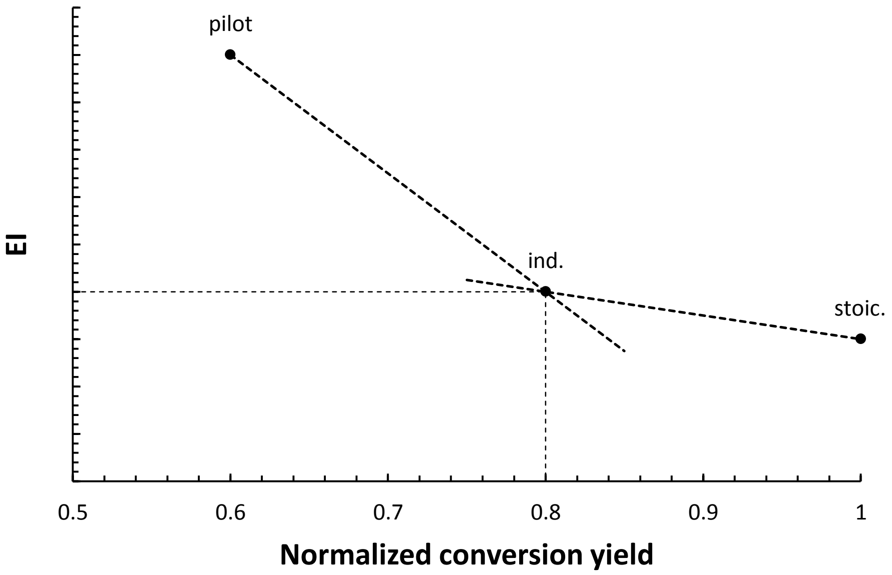


Figure 4.6 - Intersection of the scale-up functions applied to the biobased polymer

The method described above can be applied straightforwardly to a larger set of data points, considering one pair of minimum subsets (as defined in (4.5) and (4.7)) per time. This way, the resulting environmental impact of the biopolymer on an industrial scale is defined not just by one number, but by means of a values distribution that is representative of the forecast uncertainty.

4.6 RESULTS

The iteration of the procedure just described gave rise to a considerable number of results. For example, in Figure 4.7 the resulting linear interpolation for GW emissions of PET is presented.

Because of the large number of data points, the scale-up function is not limited to just one polygonal chain, but to a bundle of lines (gray area in Figure 4.7). Each scale-up function was then applied singularly to the data points representing the environmental impact of PBS, at the pilot and stoichiometric scalea. The intersections of the resulting functions identified the GW emissions of PBS produced from bio-based succinic acid (Figure 4.8).

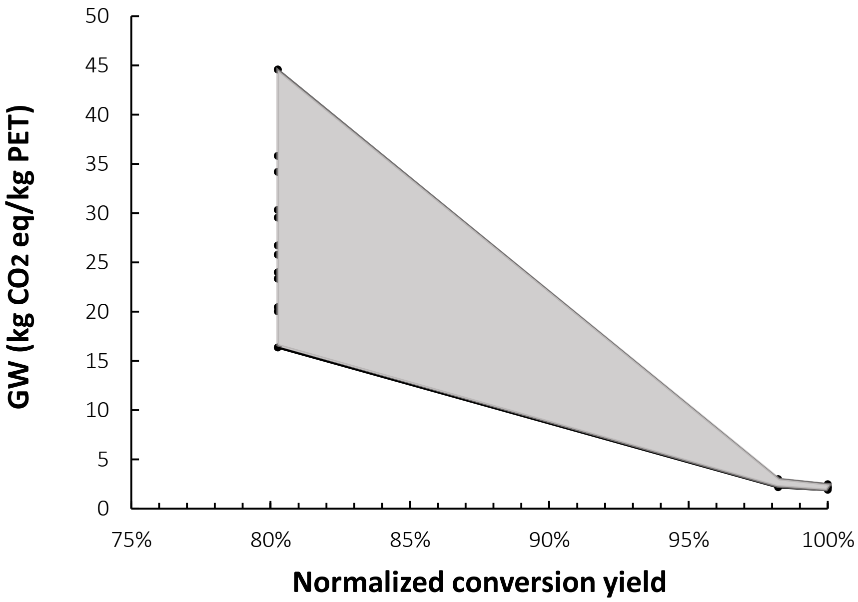


Figure 4.7 - Linear interpolation of PET data points for GW at different production scales

Following the same methodology, the CED for bio-based PBS produced on an industrial scale was assessed. Finally, the probability distribution of results for GW impact of PBS is presented in Figure 4.9 and Figure 4.11.

Furthermore, it is evident how the environmental burden of both PET and PBS on pilot scale is far higher than the respective industrial scale impact and, therefore, a direct comparison among processes at different scales would lead to inconsistent results. All of the results (mean values) for both PET and PBS are summarized in Table 4.4 and Table 4.5.

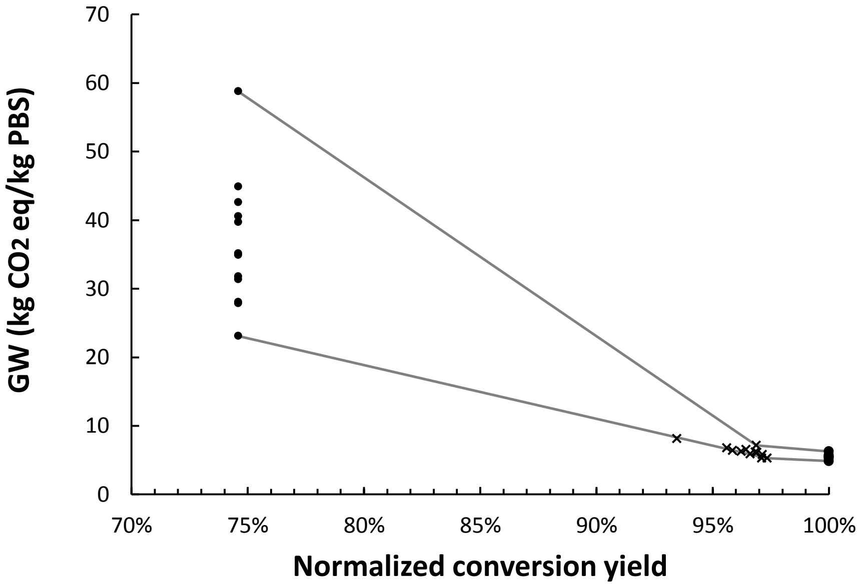


Figure 4.8 - GW impact of PBS at different production scales.

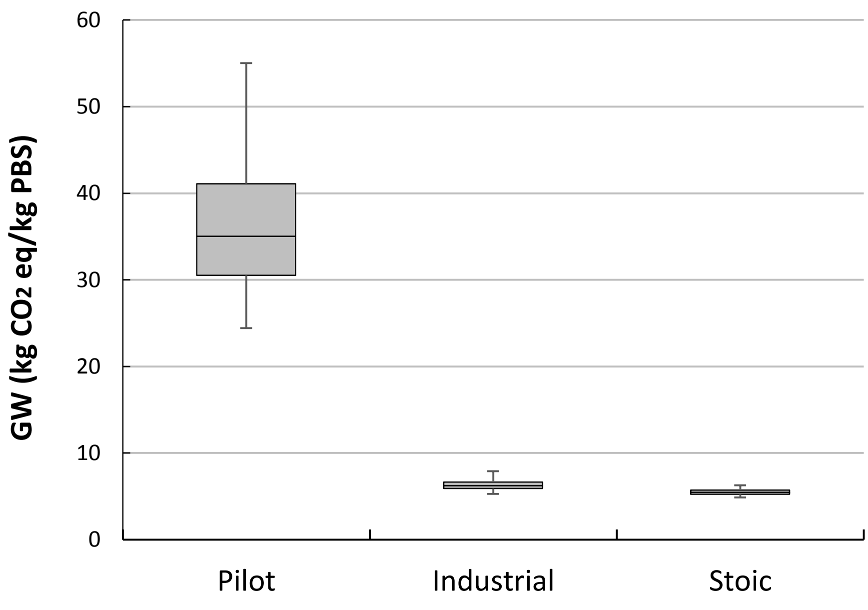


Figure 4.9 - GW impact of 1 kg of PBS (probability distributions, 5th, 25th, 50th, 75th, 95th percentiles) at different scales (pilot, industrial, stoichiometric).

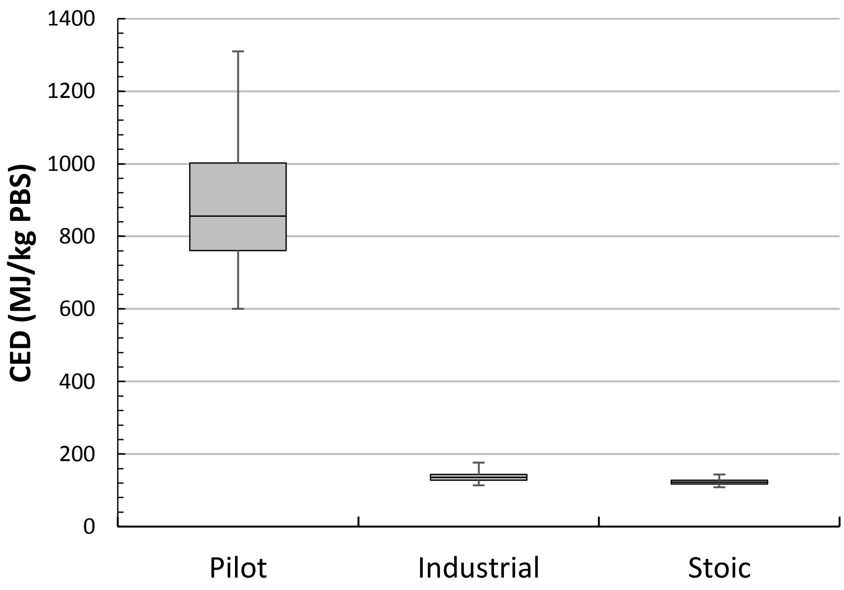


Figure 4.10 - CED for 1 kg of PBS (probability distributions, 5th, 25th, 50th, 75th, 95th percentiles) at different scales (pilot, industrial, stoichiometric).

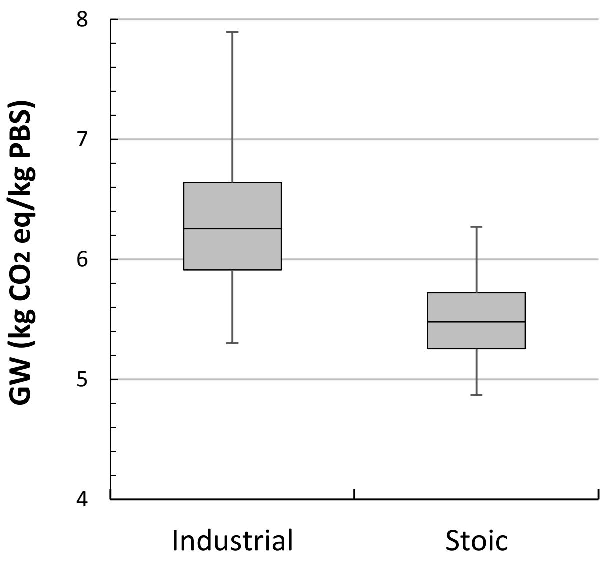


Figure 4.11 - Focus: GW impact of 1 kg of PBS (probability distributions, 5th, 25th, 50th, 75th, 95th percentiles) at different scales (industrial, stoichiometric)

Table 4.4 - Environmental impact of PET at different production scales (mean values).

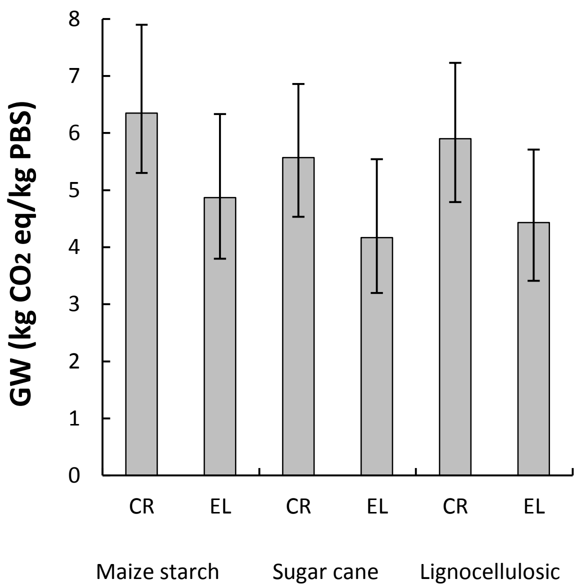
Production scale PET	CED (MJ/kg PET)	GW (kg CO_2 eq/kg PET)
Pilot	625.63	23.98
Industrial	75.71	2.54
Stoichiometric	69.05	2.15

Table 4.5 - Environmental impact of PBS at different production scales (mean values).

Production scale PBS	CED (MJ/kg PBS)	GW (kg CO_2 eq/kg PBS)
Pilot	893.55	36.57
Industrial	**138.85**	**6.35**
Stoichiometric	123.30	5.50

4.6.1 Sensitivity analysis of bio-based succinic acid

The results of the sensitivity analysis performed to evaluate the different renewable sources and production routes of the succinic acid monomer are presented in Figure 4.12. The values refers to the impact of 1 kg of PBS pellet obtained starting from the 6 different alternatives for the bio-based succinic acid. As for all of the other assessments, Monte Carlo analysis was used to cope with the uncertainty of the results and the error bars in Figure 4.12 indicate the 5th and the 95th percentile.



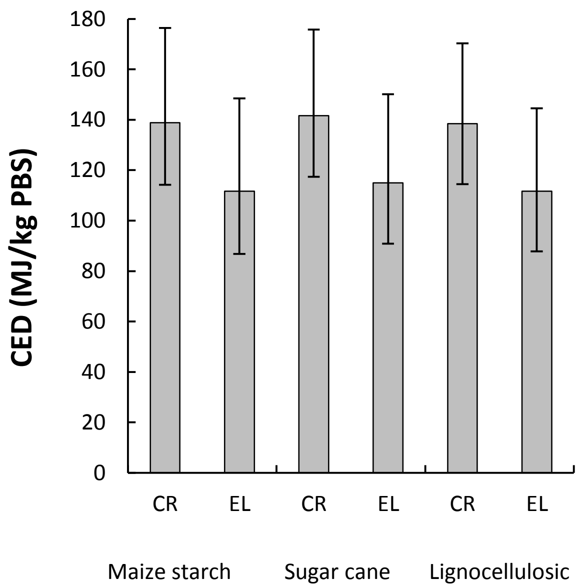


Figure 4.12 - Sensitivity analysis of GW and CED indicators for PBS with succinic acid from different renewable biomasses (maize starch, sugar cane, lignocellulosic biomass) and from different processes (CR = crystallization, EL = electrodialysis).

4.7 Discussion

For PET, the highest environmental burden occurs at the pilot scale due to the high inefficiencies present in a laboratory/pilot plant. At the industrial scale, the quality and reliability of inventory data are remarkable because the processes involved are highly optimized with the BAT and the operative conditions of the reaction are very close to the ideal stoichiometric case. This leads to a much lower environmental impact in terms of both CED and GW. Furthermore, the implementation of Monte Carlo analysis highlights a reduction in the uncertainty of results moving from the pilot scale to the industrial scale.

The results obtained by applying the scale-up protocol to the case of partly bio-based PBS are in accordance with the previous statement. With a confidence interval of 90%, we can forecast CED and GW for a future industrial production of PBS characterized by the use of BAT.

This approach clearly demonstrates that the environmental burden of a material at the pilot scale is characterized by high uncertainty and is generally far higher than the respective industrial scale impact. Therefore, a direct comparison among processes at different scales would lead to inconsistent results.

In absolute terms, both the CED and GW indicators scored higher values in the case of PBS when compared to PET on the basis of 1 kg of polymer pellet. This result does not take into account the difference in the mechanical properties of the two polyesthers. For a more consistent comparison, information on the intrinsic properties of the materials will be detailed in the next chapter.

Another relevant result derived from the linear interpolation is the forecast of the mass conversion yield that can be reached in the polymerization of PBS at the industrial scale. The estimated mass conversion yield for PBS ranges between 77.3% and 80.5%, which is lower than the mass conversion yield of the current industrial production of PET (82.7%). This result is reasonable in the light of the differing stoichiometry of the two polycondensation reactions. In fact, the maximum mass conversion yield that can be reached in ideal conditions (i.e. the stoichiometric case) for PET is 84.2%, whereas that for PBS is 82.7%.

Finally, the sensitivity analysis of the bio-based succinic acid highlights two general trends. Among the renewable sources considered, sugar cane leads to the lowest GHG emissions, followed by lignocellulosics and maize starch, whereas energy consumption is not significantly affected by the biomass source. Regarding the extraction process, electrodialysis leads to a lower environmental impact than crystallization for both of the considered indicators and independently from the starting biomass.

4.7.1 Final remarks

Life Cycle Assessment is a standardized and well developed methodology, but it still has some limitations. In particular, the reliability and consistency of results might be compromised by a production scale issue in a comparative assessment of product systems at different stages of development.

The scale-up protocol presented here aims at overcoming the scale issue arising in comparisons between innovative processes at an early stage of development and industrially optimized processes. The most relevant added value of the methodology lies in the use of primary data collected on the lab/pilot scale. Producing both the new polymer and a reference polymer in the same lab/pilot plant provides meaningful information on the actual relationship between the impacts of the two materials. A coherent model for the scale-up of the environmental burden of the new polymer can then be proposed by combining the lab/pilot data with the stoichiometric baseline.

The uncertainty analysis was performed via Monte Carlo simulations, to obtain results represented as probability density functions, rather than single deterministic values. This analysis is of particular interest in this case study, because it involved different systems (lab/pilot scale and industrial production) characterized by different efficiencies and uncertainties. This type of analysis is necessary when two alternative materials or designs have to be compared.

The case study of PBS highlights the advantages of the scale-up methodology adopted, with particular reference to ease of implementation and consistency of results. A further validation of the scale-up methodology will be performed once an Environmental Product Declaration or cradle-to-gate ecoprofile is published.

The proposed methodology could easily be applied to other biopolymers, subject to the identification of a suitable reference polymer. Furthermore, as mentioned before, the outcomes of the proposed scale-up protocol will be used for a multi-criteria comparison between bio-based PBS and traditional polymers used for food packaging, taking into account both the intrinsic properties of the materials and their environmental performance.

In the next chapter, the *ex-ante* LCA approach will be integrated with multi criteria material selection in order to better support the decision making process at the early design. This synergic integration matches the forecasted environmental performance of the bio-based polymer with its intrinsic properties and represents one of the most relevant novels of the methodologies proposed.

4.8 RESEARCH SPONSORS AND PARTNERS

This research work was supported through the THALIA project (*Produits éco-conçus pour le développement durable, validés par analyse de cycle de vie*). THALIA partners provided a valuable technical support, as well as Prof. Giovanni Camino for the scientific help and Floriane Freyermouth for the initial experiments from which it was possible to develop the scale-up protocol.

5 MULTI-CRITERIA MATERIAL SELECTION

Decisions made during the early stages of a product's design determine a significant part of its overall life cycle. In this context, materials selection is one of the most crucial choices, and designers should take into account both the mechanical/thermal/electric properties and the environmental performance of materials. When LCA is applied to a material to obtain an ecoprofile, the scope of the analysis is generally from cradle to the factory gate; furthermore, the unit of mass (or volume) of the material is usually taken as the functional unit for the analysis. However, these methodological aspects place relevant limitations on the effectiveness of the assessment. In the present work, multi-criteria analysis is used to combine the environmental performance estimated with the ex-ante LCA approach with the intrinsic properties of the materials of interest to better develop materials selection. Life Cycle Thinking is here extended to a multi-disciplinary life cycle approach.

5.1 RESEARCH QUESTION

The motivation for this research is driven by the fact that at an early stage of design, an engineering problem is set (requirements and constraints), but the solution cannot be completely defined because of the many possible scenarios still open to explore. Therefore, the research question that this work addresses is whether applying multi-criteria analysis may provide a way to innovate and support the Ecodesign process. The multi-criteria materials selection approach is here applied to the case of the previously described partly bio-based PBS, used for packaging applications. Thus, it must take into consideration the following:

- The potential environmental impacts obtained by a customized ex-ante LCA for an innovative material, including the uncertainty analysis of the results;
- A new concept of the system boundary of the environmental assessment: moving from a cradle-to-gate horizon to a cradle-to-function system.

5.2 METHODOLOGY

Multi-criteria materials selection was implemented with LCA to extend the system boundaries of the analysis and empower a comprehensive comparison among alternative materials. When LCA is applied to a material to obtain an *ecoprofile*, the scope of the analysis is generally from cradle to the factory gate. An ecoprofile typically includes raw materials extraction and conversion into semi-finished products phases. Moreover, the unit of mass (or volume) of material is usually taken as functional unit for the analysis. However, this kind of functional unit does not describe the function that a material will perform when applied in a component, but rather refers to the material production process.

These methodological limits undermine the effectiveness of the assessment (Reap et al. 2008; Finnveden et al. 2009), particularly in the case of a comparison among different materials, whose overall performances cannot be expressed in terms of unit of mass.

The approach used hereby aims at overcoming these limitations and has its turning point in the shift from a "kilogram-based" analysis to a function-oriented assessment. This change in paradigm passes through the adoption of appropriate *material indices* that include LCA results. Once identified, these indices were used in combination with *bubble diagrams* for a proper screening of the available alternatives.

5.2.1 Target

This work aims at assessing the impact of a PBS application using a multi-disciplinary life cycle approach. The adopted method synergically combines environmental results obtained by the customized *ex-ante* LCA with multi-criteria analysis for materials selection. Therefore, provided a specific function to fulfill, a comprehensive and consistent comparison between an emerging material and "traditional" materials was exploited. This multi-criteria materials selection approach was applied to the case of PBS used for packaging applications.

5.2.2 Case study

A series of design strategies have been already undertaken to mitigate the environmental impact associated with the packaging of goods. Bio-based polymers and biodegradable polymers have gained relevant attention as potential substitute materials to optimize the environmental performance of packaging solutions. In this regard, the approach here proposed was applied to PBS in order to verify and validate the environmental viability of its usage in packaging films.

In the previous chapter, a scale-up protocol for a customized ex-ante environmental impact assessment of innovative materials was developed. The ex-ante LCA approach was proposed in order to forecast the environmental burden of PBS for which process data at industrial level are not yet available.

Then, PBS used for a specific application was compared with the most common packaging polymers, i.e. low density polyethylene (LDPE), high density polyethylene (HDPE), polypropylene (PP, both high flow and low flow), polyethylene terephthalate (PET, both amorphous and semi-crystalline), polybutylene terephthalate (PBT) and polylactic acid (PLA). This comparison includes polyolefins, fossil-based polyesters and a bio-based polyester that have a wide range of mechanical properties and are produced through different chemical routes. It follows that a kilogram-based environmental comparison may lead to inconsistent and incomplete results.

Therefore, the first step of the procedure was the proper definition of the engineering problem that resulted in the identification of the most suitable *material indices*. In particular, it was modelled a thin film of material undergoing a uniaxial planar tensile stress. The mechanical properties included in the model are Young modulus (Y), tensile strength at break (σ_f) and elongation at break (ε), while the environmental performance is represented by CED and GW impact categories.

Data on the mechanical properties of PBS were retrieved both from direct measurements and from the scientific literature. In particular, tensile tests were performed on lab-scale PBS and on commercial PBS Enpol 4560J produced by IRe Chemical Ltd. Primary data were implemented with data from the datasheets of Enpol 4560J and Bionolle 1001 from Showa Denko. Data on the environmental impacts of PBS resulted from the cited ex-ante LCA, while data relating to the alternative polymers included in the comparative analysis were obtained from the database embedded in the software CES 2014 from Granta Design. An overview on all the data used is presented in Table 5.1.

Table 5.1 - Summary of mechanical and environmental data for the materials considered in the case study.

	Density (g/cm^3)	Modulus (MPa)	Tensile strength at break (MPa)	Elongation at break (%)	GW (kg CO_2 eq/kg)	CED (MJ/kg)
PBS MS CR	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	5.30 - 7.90	114.17 - 176.37
PBS MS EL	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	3.80 - 6.33	86.77 - 148.43
PBS SC CR	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	4.53 - 6.86	117.37 - 175.81
PBS SC EL	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	3.20 - 5.54	90.86 - 150.18
PBS LI CR	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	4.79 - 7.23	114.53 - 170.31
PBS LI EL	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	3.41 - 5.71	87.83 - 144.57
PBS Fossil	1.26	308.4 - 505.0	42.6 - 60.5	501.4 - 685.0	6.96 - 9.54	111.42 - 171.79
PLA	1.24 - 1.27	3300 - 3600	47 - 70	2.5 - 6	3.43 - 3.79	49 - 54.2
HDPE	0.952 - 0.965	1070 - 1090	22.1 - 31	1200 - 1290	2.64 - 2.92	77 - 85.1
LDPE	0.917 - 0.932	172 - 283	13.3 - 26.4	100 - 650	3.29 - 3.64	79.1 - 87.5
PP (high flow)	0.898 - 0.908	1370 - 1580	22.5 - 33.5	52.1 - 232	1.89 - 2.08	71 - 78.4
PP (low flow)	0.899 - 0.908	1340 - 1590	33 - 42.9	168 - 598	1.89 - 2.08	71 - 78.4
PET (amorphous)	1.29 - 1.39	2800 - 3000	55 - 60	280 - 320	3.76 - 4.15	80.9 - 89.5
PET (semi-crystalline)	1.37 - 1.4	2760 - 3100	70 - 75	65 - 75	3.76 - 4.15	80.9 - 89.5
PBT	1.30 - 1.38	1930 - 3000	56.5 - 60	50 - 300	4.67 - 5.16	94.2 - 104

MS = maize starch. SC = sugar cane. LI = lignocellulosic biomass. CR = workup via crystallization. EL = workup via electrodialysis.

5.2.3 Problem definition

The procedure leading to the identification of the material index combining tensile strength at break (σ_f) and GW is here introduced. Given the element of film presented in Figure 5.1, the design objective is to minimize the greenhouse gases emissions preserving the ability of the film to carry the load F.

Figure 5.1 - Element of film undergoing a uniaxial load.

The GW associated with the element of film (GW_{film}) that has to be minimized is given by:

$$GW_{film} = GW \cdot m = GW \cdot w \cdot t \cdot l \cdot \rho \tag{5.1}$$

where GW is the impact category describing the greenhouse gases emissions per unit of mass of material, w is the width of the element of film, t is the thickness of the element of film, l is the length of the element of film and ρ is the density of the material. At the same time, the requirement that the material must satisfy to sustain the load F is expressed by the following condition:

$$\frac{F}{w \cdot t} \leq \sigma_f \tag{5.2}$$

Considering the film thickness t as a free variable and a system of equations (5.1) and (5.2), it is possible to describe the *performance parameter* by means of the following inequality:

$$GW_{film} \geq F \cdot l \cdot \frac{GW \cdot \rho}{\sigma_f} \tag{5.3}$$

Equation (5.3) is the *objective function* for the specific engineering problem here presented: the design objective is to minimize GW_{film} that is subjected to the condition expressed in (5.3) in order to guarantee the ability of the film to support the load F. In the hypothesis that both the load F and the geometric term l are given by the problem constraints and requirements, the minimization of the performance parameter can be obtained minimizing the material-related term of (5.3) or, alternatively, maximizing its reciprocal, i.e. the *material index* MI:

$$\max_{i \in \mathbb{M}} \left(\frac{\sigma_f}{GW \cdot \rho} \right)_i \tag{5.4}$$

where the subscript i indicates the i^{th} material within the discrete set of alternative materials $\mathbb{M}$. The same procedure was performed to identify all the *material indices* considered in the present case study that are summarized in Table 5.2.

Table 5.2 - Material indices identified for the case study.

	GW	CED
Tensile strength	$\frac{\sigma_f}{GW \cdot \rho}$	$\frac{\sigma_f}{CED \cdot \rho}$
Elongation at break	$\frac{\varepsilon}{GW \cdot \rho}$	$\frac{\varepsilon}{CED \cdot \rho}$
Young modulus	$\frac{Y}{GW \cdot \rho}$	$\frac{Y}{CED \cdot \rho}$

The maximization problem formulated in (5.4) can be graphically addressed using bubble diagrams, that represent a powerful tool for a quick and visual comparison among the alternative materials belonging to the set $\mathbb{M}$. Each *material index* defines a maximization problem and corresponds to a bubble diagram whose axes are respectively the numerator and the denominator of the index itself. Taking, for example, the index $\frac{\sigma_f}{GW \cdot \rho}$, the resultant bubble diagram is presented in Figure 5.2. On a bubble diagram it is possible to identify the locus of points L where the *material index* MI is constant, i.e. to visually recognize the bubbles representing the materials which equally fulfill the design objective. The mathematical description of this set of points is:

$$L = \{(x, y) \mid MI = const\} \tag{5.5}$$

In the case of the maximization problem shown in (5.4), this can be rewritten as:

$$L = \left\{(x, y) \mid \frac{\sigma_f}{GW \cdot \rho} = const\right\} \tag{5.6}$$

Since the axes of bubble diagrams are characterized by a logarithmic scale, the condition presented in (5.6) can be reformulated as:

$$\log_{10} \sigma_f - \log_{10}(GW \cdot \rho) = const \tag{5.7}$$

Equation (5.7) describes a sheaf of parallel lines that can be superimposed on the bubble diagram and that are called *iso-performance lines*. Taking a single *iso-performance line* belonging to the sheaf, all the points on this line are characterized by the same value of the *material index*. It follows that the bubbles lying on the same line represents the materials with an equivalent eco-mechanical performance (with reference to tensile strength and GW for the particular case of Figure 5.1). At the same time, moving upwards perpendicularly to the iso-performance lines, the value of the *material index* increases and, consequently, the performance parameter (GW_{film}) decreases. As far as the optimization problem detailed hereinbefore is concerned, there is an increase of the value of $\frac{\sigma_f}{GW \cdot \rho}$ and a reduction of the value of GW_{film} moving upwards perpendicularly to the sheaf of *iso-performance lines*. The relative graphical representation is provided in Figure 5.2, where an iso-performance line is highlighted, as well as the direction along which the eco-mechanical performance increases.

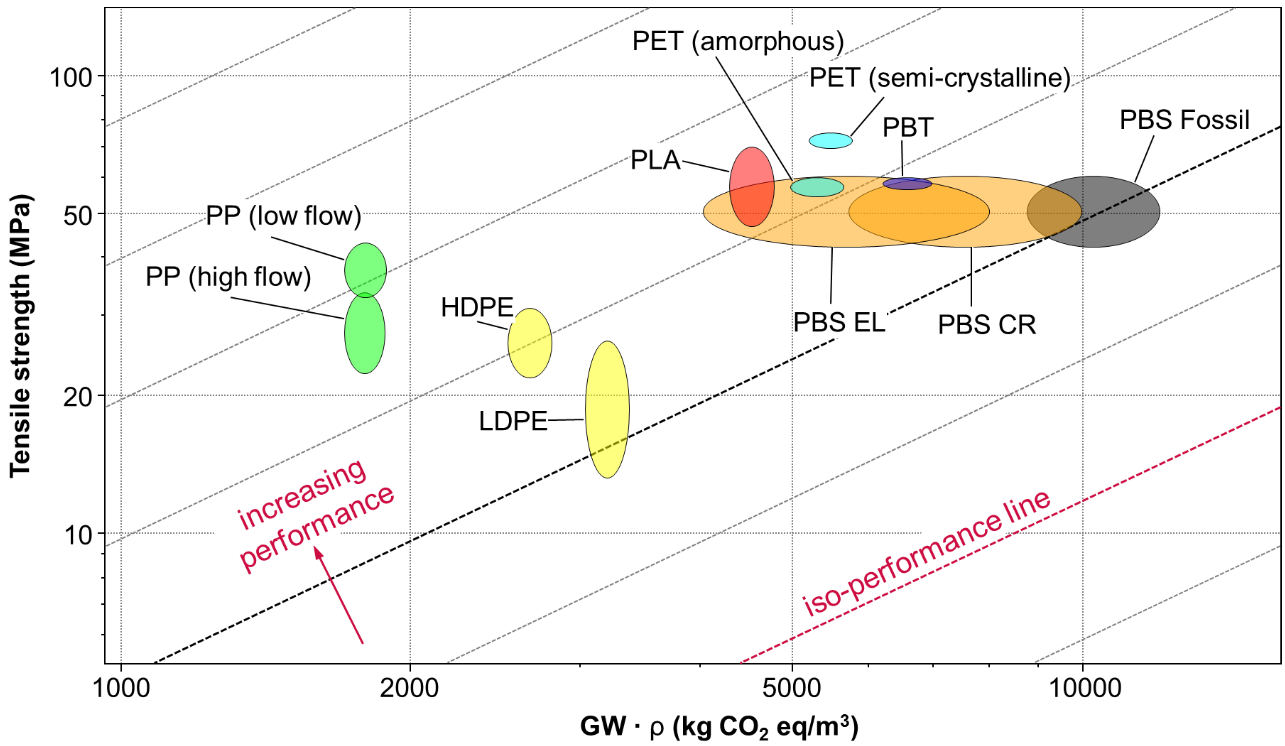


Figure 5.2 - Ashby plot for a materials selection based on the material index $\frac{\sigma_f}{GW \cdot \rho}$

5.3 Results

The procedure detailed in the previous section was applied for all the 6 relevant material indices that were identified in order to evaluate the viability of the usage of partly bio-based PBS in packaging films. The 6 resulting Ashby plots are presented in Figure 5.3 to Figure 5.8.

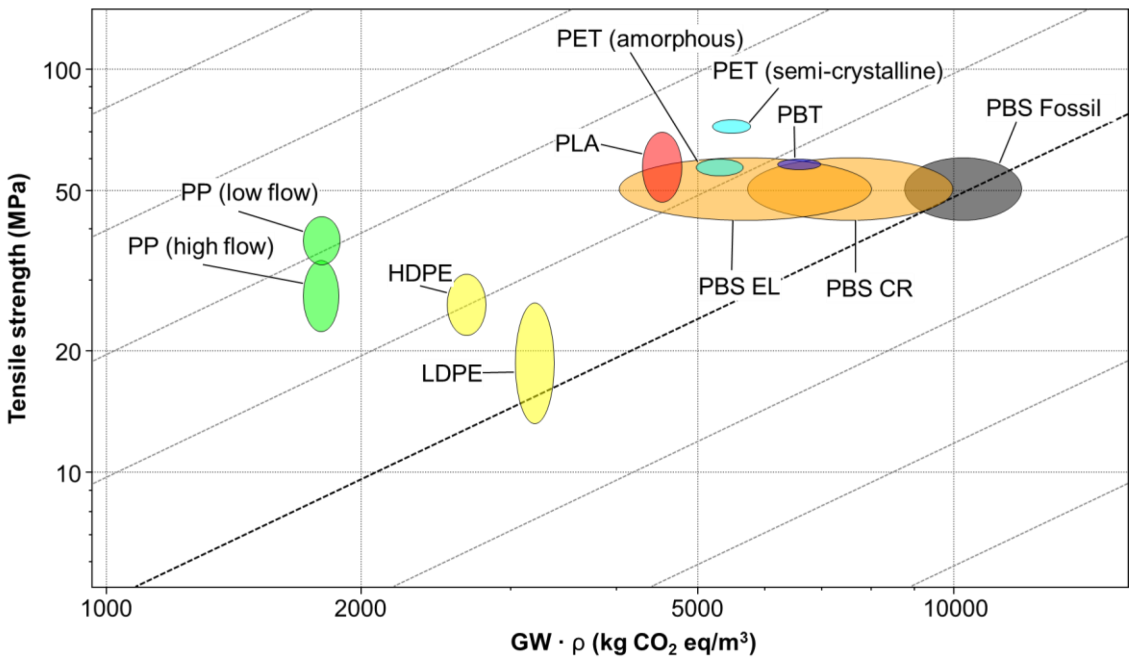


Figure 5.3 - Ashby plot for materials selection based on the material index σ_f vs $GW \cdot \rho$

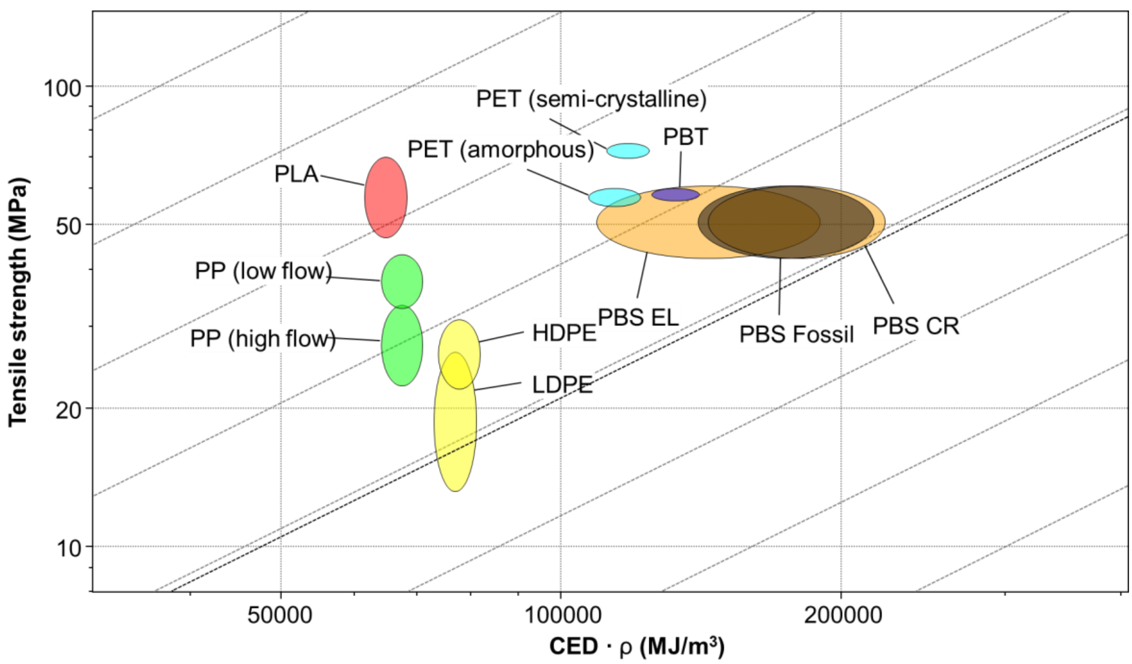


Figure 5.4 - Ashby plot for materials selection based on the material index σ_f vs $CED \cdot \rho$

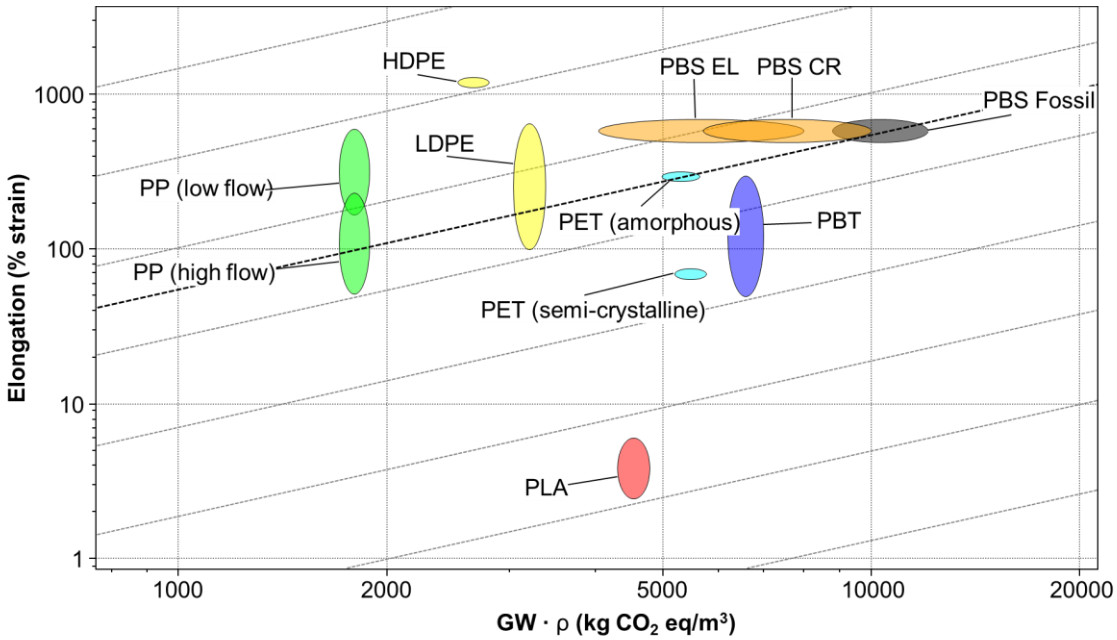


Figure 5.5 - Ashby plot for materials selection based on the material index ε vs $GW \cdot \rho$

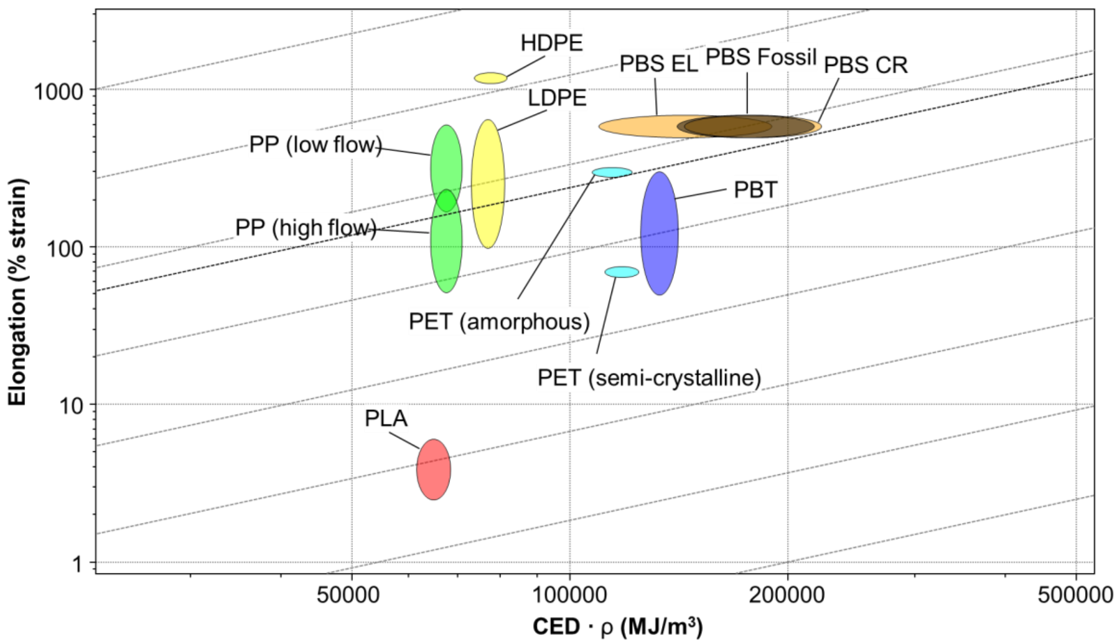


Figure 5.6 - Ashby plot for materials selection based on the material index ε vs $CED \cdot \rho$

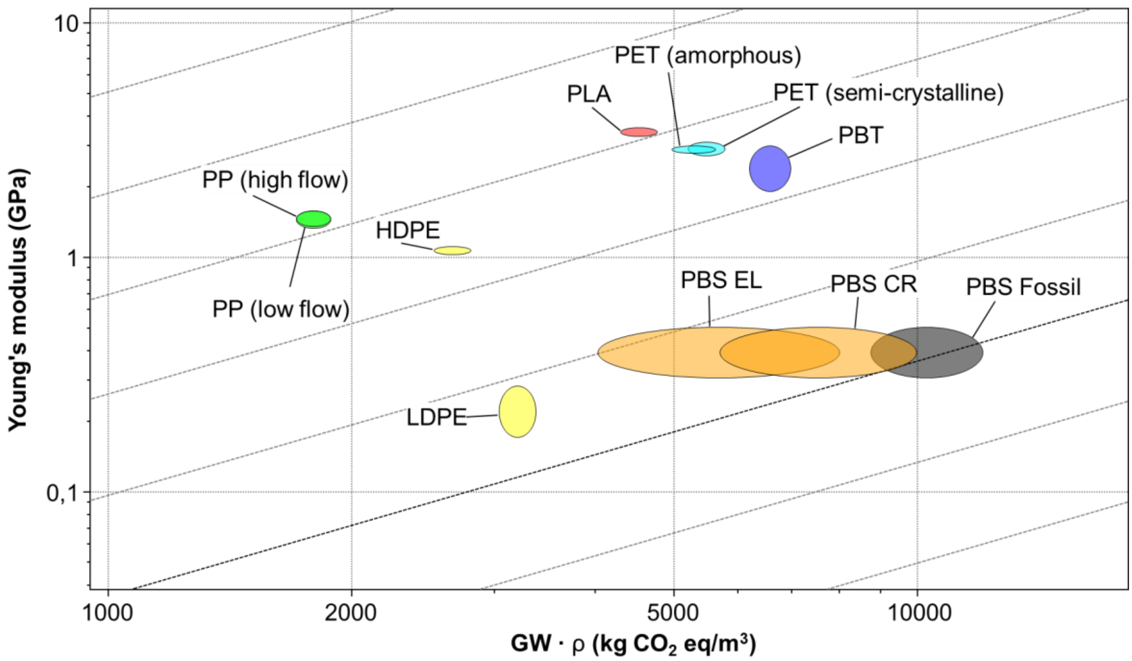


Figure 5.7 - Ashby plot for materials selection based on the material index Y vs $GW \cdot \rho$

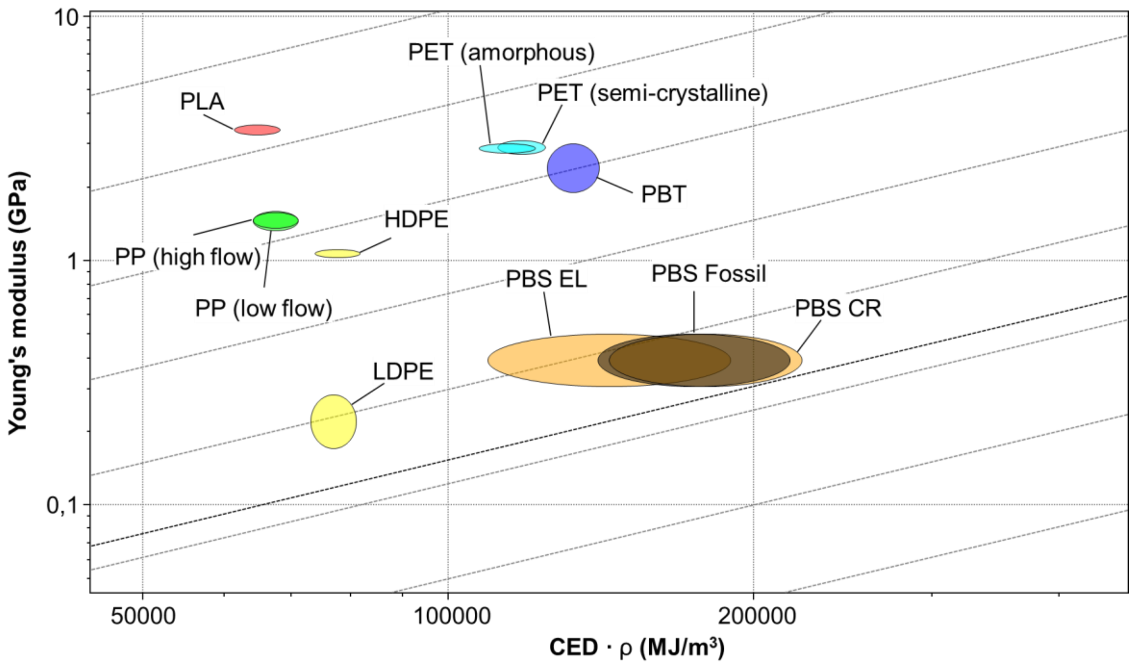


Figure 5.8 - Ashby plot for materials selection based on the material index Y vs $CED \cdot \rho$.

As far as partly bio-based PBS is concerned, the results of the 6 alternatives considered in the sensitivity analysis were classified in 2 categories according to the possible workup routes, i.e. crystallization (PBS CR) and electrodialysis (PBS EL).

Considering tensile strength with respect both to GW and CED, PBS bubbles are located in an iso-performance region that includes most of the alternatives. In particular, focusing on σ_f versus $GW \cdot \rho$, PBS has a performance equivalent to the polyesters and polyethylenes, while it is slightly outranked by the polypropylenes. In the case of σ_f versus $CED \cdot \rho$, PLA performs above all the other material, followed by PP and PET, while PBS is in line with the other alternatives. Looking at the elongation at break both in the case of $GW \cdot \rho$ and $CED \cdot \rho$, PBS shows a widely better performance than other polyesters and is comparable with the polyolefins considered. Finally, as far as the Young's modulus is concerned, PBS is outranked by all the other polymers, with the exception of LDPE.

Narrowing the scope of the comparison to the PBS options, oil-based PBS performs clearly worse than bio-based alternatives when GHG emissions are considered (GW indicator), whereas it is characterized by a CED similar to the CED of partly bio-based PBS obtained through crystallization. In general, electrodialysis is the preferable chemical route for producing the succinic acid monomer from renewable sources.

5.3.1 Oxygen permeability

Focusing on the functions to be fulfilled by a packaging film, the oxygen permeability is one of the most relevant material property. In particular, food packaging must be designed to meet a series of requirements. The primary requirement is food protection from the external environment and long-lasting preservation. These features are of major importance in influencing customers behavior and buying preferences (Löfgren and Witell 2005).

Given the previous considerations, the case study here implemented (packaging film for food) must concern data on oxygen permeability for the alternative materials considered in order to guarantee a comprehensive eco-selection. The oxygen permeability of PBS packaging film is shown in Figure 5.9 in comparison with the other alternatives. Data on the oxygen permeability of PBS were retrieved from Okamoto et al., (2003). Density is included because the design aims at mass minimization as it leads to environmental impact reduction.

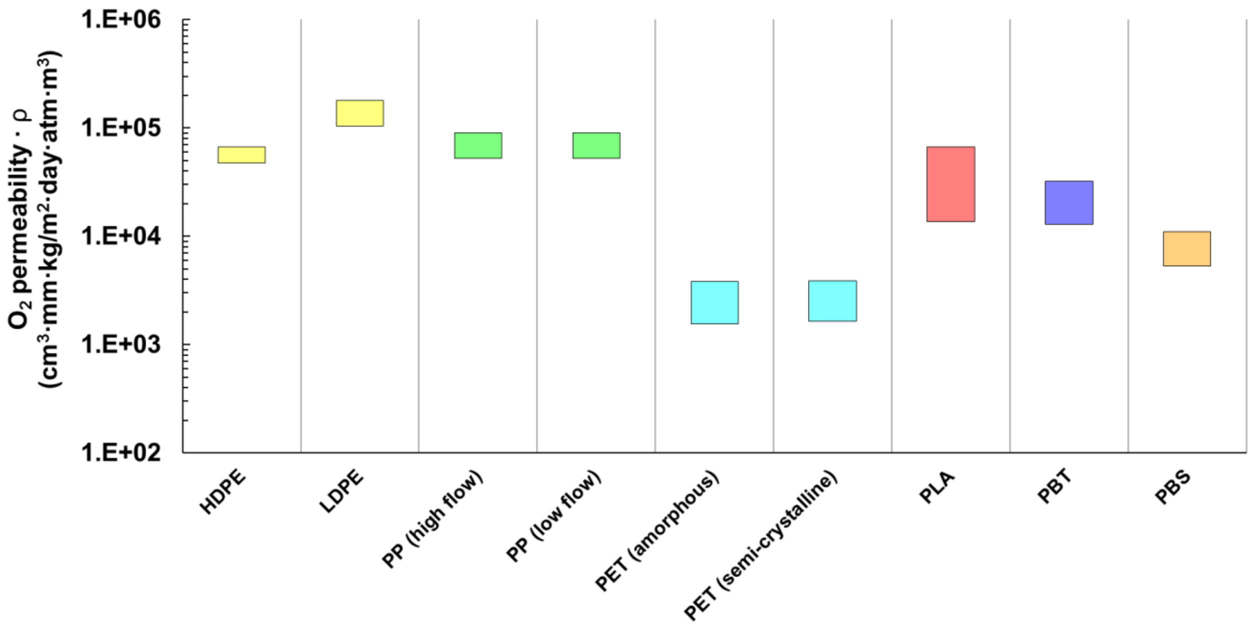


Figure 5.9 - Values of O_2 $permeability \cdot \rho$ for the polymers considered in this case study.

The best performance is reached by PET, that presents the lowest value of oxygen permeability, followed by PBS, while all the other alternatives have poorer barrier properties. Finally, a multi-criteria comparison was performed combining the oxygen permeability with the *material index* concerning elongation at break and GW.

In particular, $O_2\ permeability \cdot \rho$ was plotted against the reciprocal of $\frac{\varepsilon}{GW \cdot \rho}$ (Figure 5.10) and $\frac{\varepsilon}{CED \cdot \rho}$ (Figure 5.11). In the resulting Ashby plot, the closer the material bubble is to the origin of the axes, the better is its performance for both the indices considered. In fact, moving towards the origin of the axes, the oxygen permeability is minimized and material indices are simultaneously maximized.

As it generally happens in multi-criteria decision processes, there is no solution that optimizes all of the criteria at the same time, providing one single optimal choice. However, it is possible to identify a set of alternatives (in this case a set of materials) representing the best trade-offs; these alternatives are called *non-dominated* solution. All the others options are called *dominated* since there is at least one alternative that performs better in one criterion without detriment to the other criterion.

In the cases of Figure 5.10 and Figure 5.11, the set of *non-dominated* solutions includes HDPE, PBS EL and PET (amorphous) options.

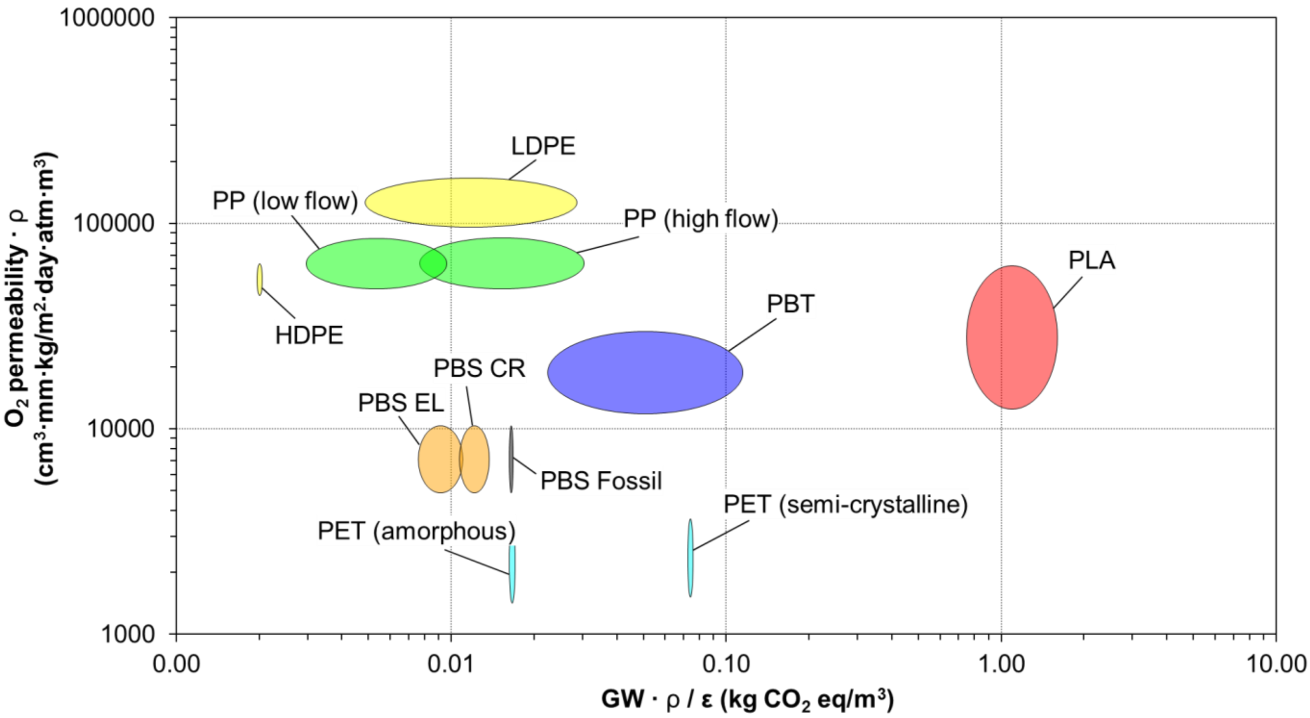


Figure 5.10 - Ashby plot for the multi-criteria materials selection based on $O_2\ permeability \cdot \rho$ *and* $\frac{\varepsilon}{GW \cdot \rho}$.

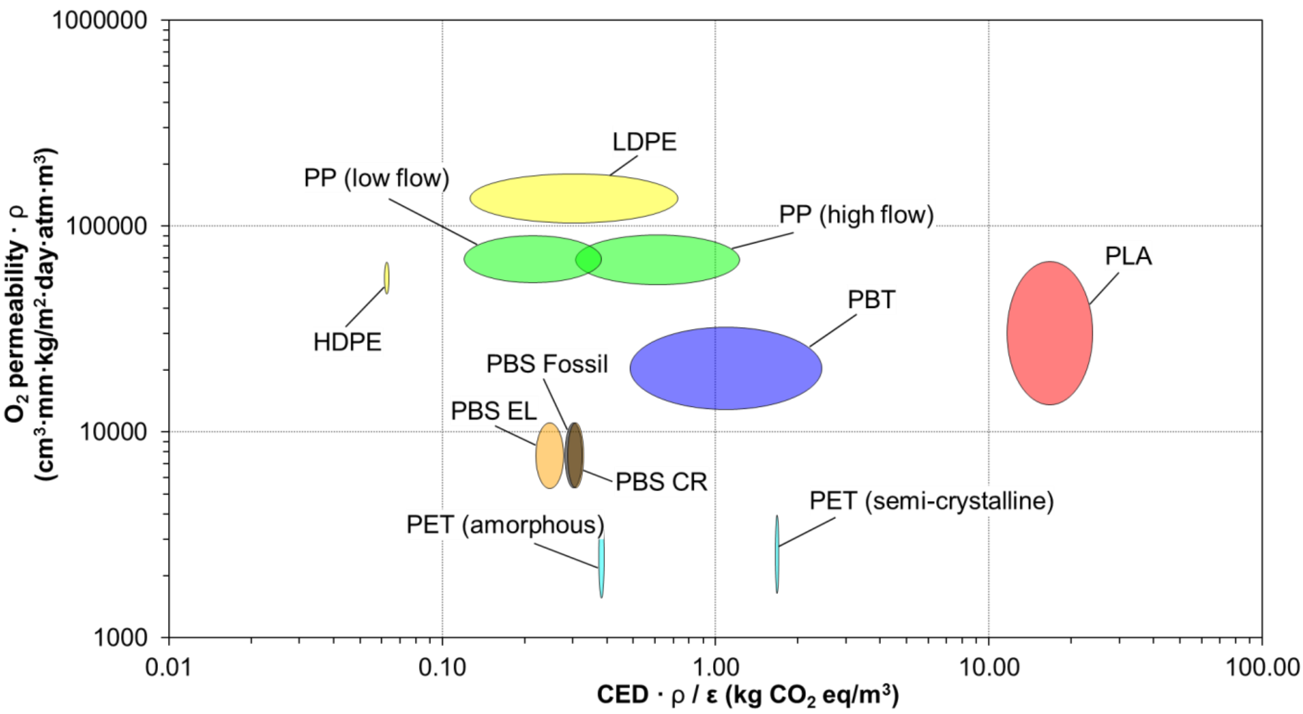


Figure 5.11 - Ashby plot for the multi-criteria materials selection based on $O_2\ permeability \cdot \rho$ *and* $\frac{\varepsilon}{CED \cdot \rho}$.

5.4 DISCUSSION

When deciding to substitute bio-based plastics for conventional petroleum-based plastics, it is important to understand the flow of these materials and their impacts in all phases of their life cycles to select a material that is more suitable (Álvarez-Chávez et al. 2012). The analysis conducted by Álvarez-Chávez et al. (2012) found that none of the analyzed bio-based polymers, currently in commercial use or under development, is fully sustainable. It is also challenging to address requirements such as naturalness and high quality through bio-based materials, as demonstrated by Karana (2012).

The results obtained in the present work are coherent with these previous findings. In fact, partly bio-based PBS proved to be comparable to the most commonly used packaging polymers, but the environmental benefits are not straightforwardly guaranteed by the renewable origin of the monomers. However, the combination of mechanical performance, barrier properties, and environmental burden makes PBS a viable option for packaging film applications, particularly as an alternative to polyolefins.

From the Ashby plots analysis, partly bio-based PBS performed comparably to PE for all the *material indices* and, in addition, it was characterized by considerably better barrier properties. At the same time, if compared to other polyesters, the higher elongation at break of PBS is beneficial in the case of films, because it ensures the packaging integrity to a larger extent of deformation. This is particularly evident in the multi-criteria comparison represented in Figure 5.10 and Figure 5.11: considering GW, for instance, the set of non-dominated solutions includes HDPE, because it is the best option for the maximization of $\frac{\varepsilon}{GW \cdot \rho}$; PET (amorphous), because it is the best option for the minimization of the oxygen permeability, and PBS EL, because it is the best trade-off of the two characteristics.

Furthermore, it is important to recall that a proper LCA study requires a holistic approach and therefore, in the specific case here analyzed, it is advisable to consider not only the packaging itself but rather the overall product-packaging system (Williams et al. 2008). If the product is food, the analysis must include those elements that may affect the food's shelf life and, eventually, the production of food leftovers and food waste (Williams and Wikström 2011). Williams and Wikström (2011) showed that in some cases, an increase in the environmental burden of the packaging may result in a reduction of food waste and ultimately in a reduction of the overall environmental impact of the relative food-packaging system. This is very likely to happen in the case of PBS packaging, which could extend the shelf life of some food products (Breedveld et al. 2014) because PBS has adequate barrier properties, especially regarding oxygen permeability. This feature is particularly useful in the case of primary food packaging. At the same time, the high elongation at break exhibited by PBS is of relevant interest if used for secondary packaging.

As far as the approach here presented is concerned, the use of a *material index* as a functional unit for the environmental assessment leads to more comprehensive results with respect to a kilogram-based evaluation. Actually, if CED and GW are referred to the unit of mass, partly bio-based PBS presents a higher impact compared to fossil polyolefins. This is mainly due to a different polymerization process and a different consumption of energy. Moreover, the mechanical properties are different. In particular, the higher mechanical performances of PBS allows a reduction of the component mass, without compromising the fulfilment of its function. It follows that a smaller mass of material needed for the component is translated into an overall decrease of the environmental impact of the component itself.

This leads to conclude that functionality should be combined with environmental results to support a comprehensive materials selection.

5.4.1 Final remarks

In the present work, the authors applied a combined approach to perform a comprehensive comparison in the context of a change-oriented materials selection aimed at the optimization of the eco-mechanical performance of a packaging film. In particular, the proposed approach combines an *ex-ante* LCA, uncertainty analysis and the multi-criteria materials selection process based on the Ashby methodology.

Here, PBS proved to be competitive with other fossil-based polymers thanks to a combination of properties related to the environmental impact, relevant mechanical properties, and barrier properties. In fact, considering all of these properties with a multi-criteria approach, PBS films rank among the best trade-offs.

The results of the case study provided validation of the effectiveness and suitability of this approach in assessing the environmental burden of newly developed bio-based polymers. One of the key points of this research is the inclusion of non-environmental properties of the material in the functional unit by means of *material indices*. This shift in the functional unit allows an expansion of the system boundaries from a *cradle-to-gate* horizon to a *cradle-to-function* framework. This approach is intended to avoid possibly misleading interpretations of results when comparing materials on the basis of only their ecoprofiles.

Finally, the use of material indices as functional units for LCA of materials displayed great potential that goes beyond the scope of the present work and needs to be explored for other materials in future works.

6 CONCLUSIONS

The work presented in this thesis was aimed at streamlining a complex process, specifically an LCA study. From a methodological point of view, the most recognized weaknesses of LCA are turned into points of strength for streamlined approaches:

- The need for characterization of uncertainty in LCA results;
- The lack of primary data for innovative or early-stage systems;
- The integration of environmental results and material properties for materials selection.

As stated by Lloyd and Ries (2008) the LCA community should develop a better understanding of the importance of different types of uncertainty and variability and develop protocols for reliably characterizing, propagating, and analyzing uncertainty in LCA. In this thesis, the uncertainty analysis represents one of the most relevant points of strength because, through a probabilistic characterization of the uncertainty in the results, it was possible to accomplish the following:

- Develop a classification of materials, a classification of assemblies, and their corresponding distributions of environmental results at different levels of specificity. Thanks to this approach, the design process can be effectively supported by LCA, even during the early stages;
- Realize a scale-up protocol for the potential environmental impacts of innovative materials. The ex-ante LCA approach allows forecasting of the distributions of results, based primarily on experiments conducted at the pilot plant scale. Through the characterization of uncertainty, cradle-to-gate results can be used in multi-criteria materials selection analyses, thereby developing cradle-to-function information that is useful for Ecodesign.

Although there are several common strategies in the case studies analyzed for this thesis, methodological differences can be highlighted as well.

Probabilistic underspecification.

- Probabilistic underspecification and probabilistic triage were focused on the application of LCA at different stages of the design process. Test results highlighted that the former approach is efficient and useful for limiting the need for data collection, though its performance depends on the assembly population: as the number of assemblies grows, the uncertainty in the results increases due to greater variation. A potential limitation in using probabilistic underspecification may be the broad uncertainty in the results for a concept or a schematic design.
- The LCA results highlighted how data dispersion can vary depending on 1) the considered level of specification and 2) the considered environmental impact category. In some cases, the trends of

the MAD-COV performance metric indicated that the uncertainty in results can increase with the specificity. These anomalies occur due to the fact that the same group of materials can be heterogeneous and characterized by different environmental profiles. At certain levels, even the comparison indicator required more detail in data specification when a significant probability of success could not be reached.

- This kind of approach is of particular interest in the United States of America because the construction sector there works in a particular way. Building designs (geometry, type of structure, etc.) are often standard, and generally, builders implement variations to meet the local building codes. Designers can therefore explore, by means of this approach, new construction techniques with a consistent number of options.

Probabilistic triage.

- To achieve results with this method effectively, a probabilistic triage is necessary. Tests conducted with the comparison indicator in support of probabilistic underspecification led to the development of a probabilistic triage approach that helps identify which components need to be specified to represent a significant part of the environmental impact of the product.
- With probabilistic triage, for a specific product, it is possible to identify a set of specific parameters of influence. If applied to a specific category of products, it can be helpful to focus attention on what really matters. Application to a category requires 1) a significant number of previous LCA studies with which to identify the set of interest for the category and 2) a study of the uncertainty in the initial quantities of materials.
- This approach can be useful for well-known product categories, such as buildings and construction materials, but also electronic products. Ongoing experiments are demonstrating how electronic devices use three main categories of materials (metals, precious metals and plastics), and specific information about materials (particularly precious metals) or components (e.g., integrated circuits) can streamline the analysis. Another area of future application will be the automotive sector. In this case, where bills of materials are already available, they include thousands of items and the LCI phase can be streamlined efficiently and effectively.

Ex-ante LCA.

- The scale-up protocol for ex-ante LCA was intended for the early-stage design of a non-conventional system that has not yet been developed at the industrial scale.
- Tests conducted with a partly bio-based polymer (polybutylene succinate) highlighted how LCA can be streamlined efficiently using the cradle-to-gate results of a similar and optimized technological

process. This test purposely avoided complex thermodynamic considerations or predictive models to preserve the efficiency of the process and avoid iterations between process engineers and life cycle analysts.

- A major limitation of this case study is the lack of a third party review of this work, as a published ecoprofile for polybutylene succinate is not yet available. For this example, it was possible to estimate a distribution of environmental results, but it is not possible to associate a confidence interval with that distribution. Therefore, future works will evaluate the effectiveness of this case study.
- In general, the scale-up protocol may face another limitation if it is not possible to find a conventional system or a similar technological process with available secondary data. However, it can be extremely useful if secondary data about best available technologies are available for use.
- The use of a unit of mass as a functional unit is often applied for materials used for different purposes (plastic granules, metals, biomasses, etc.). This approach is convenient for life cycle specialists, but the possible function of the material is not taken into account. This is why a multi-criteria analysis was developed to support materials selection.

Multi-criteria materials selection.

- The multi-criteria materials selection approach was implemented for the PBS case study using the results obtained with the ex-ante LCA. The use of multi-criteria analysis *per se* is not an innovative element, as materials selection tools allow the combination of material properties and environmental impacts. Here, the most novel element consists of the use of the customized *ex-ante* Life Cycle Assessment and the uncertainty analysis used to determine the uncertainty in material indices.
- Test results indicated that the expansion of the scope definition for ecoprofiles was particularly useful for encompassing different features of the design under development. If Life Cycle Assessment includes all of the activities involved in a single product's life cycle, this multi-disciplinary approach streamlines the comparison among several single products characterized by different properties.
- From a methodological point of view, multi-criteria materials selection appears to be the most promising tool for the immediate future. It was proven to strengthen Life Cycle Assessment for both sustainable and functional decision-making in design processes. Additionally, it is not just recommended for complex systems; if polybutylene succinate films are tested for food packaging, for instance, designers have to meet a series of requirements. The primary requirement is food protection from the external environment and long-lasting preservation. This approach can be

useful for developing better Ecodesign; it is not an option for changing the use of LCA, but rather a means of changing design management using a real multi-disciplinary life cycle approach.

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APPENDIX A - PEDIGREE MATRIX

Score:	1	2	3	4	5
1 Reliability	Verified data based on measurements	Verified data partly based on assumptions OR non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimate (e.g. by industrial expert); data derived from theoretical information (stoichiometry, enthalpy, etc.)	Non-qualified estimate
	1.00	1.05	1.10	1.20	1.50
2 Completeness	Representative data from all sites relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from >50% of the sites relevant for the market considered over an adequate period to even out normal fluctuations	Representative data from only some sites (<<50%) relevant for the market considered OR >50% of sites but from shorter periods	Representative data from only one site relevant for the market considered OR some sites but from shorter periods	Representativeness unknown or data from a small number of sites AND from shorter periods
	1.00	1.02	1.05	1.10	1.20
3 Temporal correlation	Less than 3 years of difference to our reference year	Less than 6 years of difference to our reference year	Less than 10 years of difference to our reference year	Less than 15 years of difference to our reference year	Age of data unknown or more than 15 years of difference to our reference year
	1.00	1.03	1.10	1.20	1.50
4 Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from smaller area than area under study, or from similar area	Data from area with slightly similar produc-tion conditions	Data from unknown OR distinctly different area (north America instead of Middle East, OECD-Europe instead of Russia)
	1.00	1.001	1.02	1.05	1.10
5 Further technological correlation	Data from enterprises, processes and materials under study (i.e. identical technology)	Data from processes and materials under study (i.e. identical technology) but from different enterprises	Data on related processes or materials but same technology, OR data from processes and materials under study but from different technology	Data on related processes or materials but different technology, OR data on laboratory scale processes and same technology	Data on related processes or materials but on laboratory scale of different technology
	1.00	1.05	1.20	1.50	2.00

APPENDIX B - BASIC UNCERTAINTY

input / output group C=combustion emissions, P=process emissions, A=agricultural emissions	C	P	A
Demand of:			
Thermal energy, electricity, semi-finished products, working material, waste treatment services	1,05	1,05	1,05
Transport services (tkm)	2,00	2,00	2,00
Infrastructure	3,00	3,00	3,00
Resources:			
Primary energy carriers, metals, salts	1,05	1,05	1,05
Land use, occupation	1,50	1,50	1,10
Land use, transformation	2,00	2,00	1,20
Pollutants emitted to water:			
BOD, COD, DOC, TOC, inorganic compounds (NH_4, PO_4, NO_3, Cl, Na etc.)		1,50	
Individual hydrocarbons, PAH		3,00	
Heavy metals		5,00	1,80
Pesticides			1,50
NO_3, PO_4			1,50
Pollutants emitted to soil:			
Oil, hydrocarbon total		1,50	
Heavy metals		1,50	1,50
Pesticides			1,45
Pollutants emitted to air:			
CO_2	1,05	1,05	
SO_2	1,05		
NMVOC total	1,50		
NO_X, N_2O	1,50		1,40
CH_4, NH_3	1,50		1,20
Individual hydrocarbons	1,50	2,00	
PM>10	1,50	1,50	
PM10	2,00	2,00	
PM2.5	3,00	3,00	
Polycyclic aromatic hydrocarbons (PAH)		3,00	
CO, heavy metals		5,00	
Inorganic emissions, others		1,50	
Radionuclides (e.g. Radon-222)		3,00	

Appendix C - Streamlined LCA approaches

Int J Life Cycle Assess

Table 1 Summary of streamlined approaches for life cycle-based assessments

	Description	Sustainability perspectives			Qual./Quant.	Based on case-specific data
		Envir.	Soc.	Econ.		
Hot spot analysis (Wallbaum and Kummer 2006, as cited in Bienge et al. 2010)	Elaboration of the most relevant ssues or phases influencing resource use in the life cycle/value chain	x			Quant.	x
Sustainability hot spot analysis (Bienge et al. 2010)	Elaboration of the most relevant factors or phases influencing resource use, further environmental and social impacts in the life cycle/value chain	x	x	(x)	Qual./quant.	x
Life cycle thinking	Conceptual application of life cycle-based methods	x	(x)	(x)	Qual.	x
Streamlined LCA	Preliminary, shortened LCA either qualitatively or by using readymade databases	x			Qual./quant.	(x)
7-Step approach to environmental improvement through product development (McAloone and Bey 2009)	Systematic and creative 7-step approach to identify the company's potential for creating synergy between environmental improvement and business creation	x	(x)	(x)	Qual.	x
Rules of thumb	Simple design rules based on experience from "ordinary" quantitative LCA studies, which repeatedly reveal the same environmental impact source (e.g., reduced environmental impact in transportation through lower weight)	x			Qual.	
LCA-derived proxies	Simple, easy-to-measure metrics evaluate a product with respect to its critical environmental properties. A well-known proxy is MIPS (Schmidt-Bleek 1994), calculating material weight	x			Quant.	x
Socio-ecological impact matrix, ecomatrix (Belz 2005)	Analytical tool in matrix form exhibits social and ecological problems of a life cycle: on the *x*-axis are the stages of life cycle and different ecological and social dimensions on the *y*-axis	x	x		Qual.	x
MET matrix (Brezet and van Hemel 1997)	Analytical tool in matrix form, covering main life cycle stages on the *x*-axis and main environmental impacts on the *y*-axis (material, energy, toxicity)	x			Qual./quant.	x
MECO matrix (Wenzel 1998)	Analytical tool in matrix form, covering main life cycle stages on the *x*-axis and main inputs and outputs on the *y*-axis (material, energy, chemicals, others)	x			Qual.	x
Software tools	Software packages allowing quick execution of an LCA through built-in large material and databases. Often only cradle-to-gate data.	x			Quant.	
Artificial neural network (ANN) modeling (Park et al. 2001)	"learning by example," used to perform preliminary environmental assessments. Based on what is known from existing products, ANN models are "trained" to model a new product	x			Quant.	
Combination tools (e.g., eco-functional matrix, QFD-LCA)	Combine, e.g., LCA with assessment of other aspects (e.g., technical aspect, cost), without going into too much detail	x	(x)	(x)	Quant.	x
Life cycle design structure matrix (LC-DSM) (Schlüter 2001)	Different life cycle stages are both on the *x*- and *y*-axis and the relations	x			Quant.	x

Table 1 (continued)

	Description	Sustainability perspectives			Qual./Quant.	Based on case-specific data
		Envir.	Soc.	Econ.		
	between all stages are noted in the matrix					
Environmentally responsible product assessment matrix (ERPA) (Graedel and Allenby 1995 as cited by Baumann and Tillman 2004)	Semiquantitative LCA, 5×5 matrix, one dimension is the life cycle stages and the other is environmental concern; total environmental responsibility is the sum of the matrix element values.	x			Semi-quant.	x
ESAT (Schulz et al. 2012)	Software tool using life cycle inventory data for rapid estimation of the environmental and economic performance of different water servicing scenarios which are further prioritized by interactive multicriteria analysis	x		x	Quant.	
Reverse LCA (Graedel 1998, as cited by Baumann and Tillman 2004)	Begins with the ideal environmental impacts of a product and works backward to determine the physical design satisfying them	x			Qual.	x
Carbon footprint e.g., Wiedmann and Minx 2008)	Same system boundaries and FU than LCA, but only one impact category	x			Quant.	x
Simplified GWP algorithm (Bala et al. 2010)	Calculates GWP for the most important phases in the product life cycle	x			Quant.	(x)
Simplified differences modeling (Bala et al. 2010)	Comparing recycling systems, takes into account only the differences that occur in one system vs. the other	x			Quant.	(x)

Source: Hanna-Leena Pesonen & Susanna Horn, 2012. *Evaluating the Sustainability SWOT as a streamlined tool for life cycle sustainability assessment*. International Journal of Life Cycle Assessment. DOI 10.1007/s11367-012-0456-1

APPENDIX D - ACRONYMS

AP	Acidification
BAT	Best Available Technologies
BOA	Bill Of Activities
BOM	Bill Of Materials
CV	Coefficient Of Variation
DfE	Design for Environment
ECD	Environmentally Conscious Design
EEA	Environmental Effect Analysis
EP	Eutrophication
EPD	Environmental Product Declaration
ERP	Energy Related Product
EUP	Energy-Using Product
FMEA	Failure Mode and Effect Analysis
GHG	Greenhouse gas
GW	Global Warming
GWP	Global Warming Potential
ICF	Insulated Concrete Form
INSA	Institut National des Sciences Appliquées de Lyon
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LCT	Life Cycle Thinking
MAD-COV	Median Absolute Deviation – Coefficient Of Variation
MCA	Multi-criteria Analysis
MD	Median Distance
MSL	Materials Systems Laboratory
PBS	Polybutylene succinate
PCR	Product Category Rules
POCP	Photochemical Ozone Creation Potential
SM	Photosmog creation
SOI	Set of Interest

APPENDIX E - AUTHOR'S PUBLICATIONS

Under review. Tecchio P., Freni P., De Benedetti B., Fenouillot F. (2015). Ex-ante life cycle assessment approach developed for a case study on bio-based polybutylene succinate. Journal of Cleaner Production.

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Work in progress (article). Tecchio P., Gregory J., Ghattas R., Kirchain R. (2015). Streamlining the life cycle assessment of buildings by data specification triage.

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